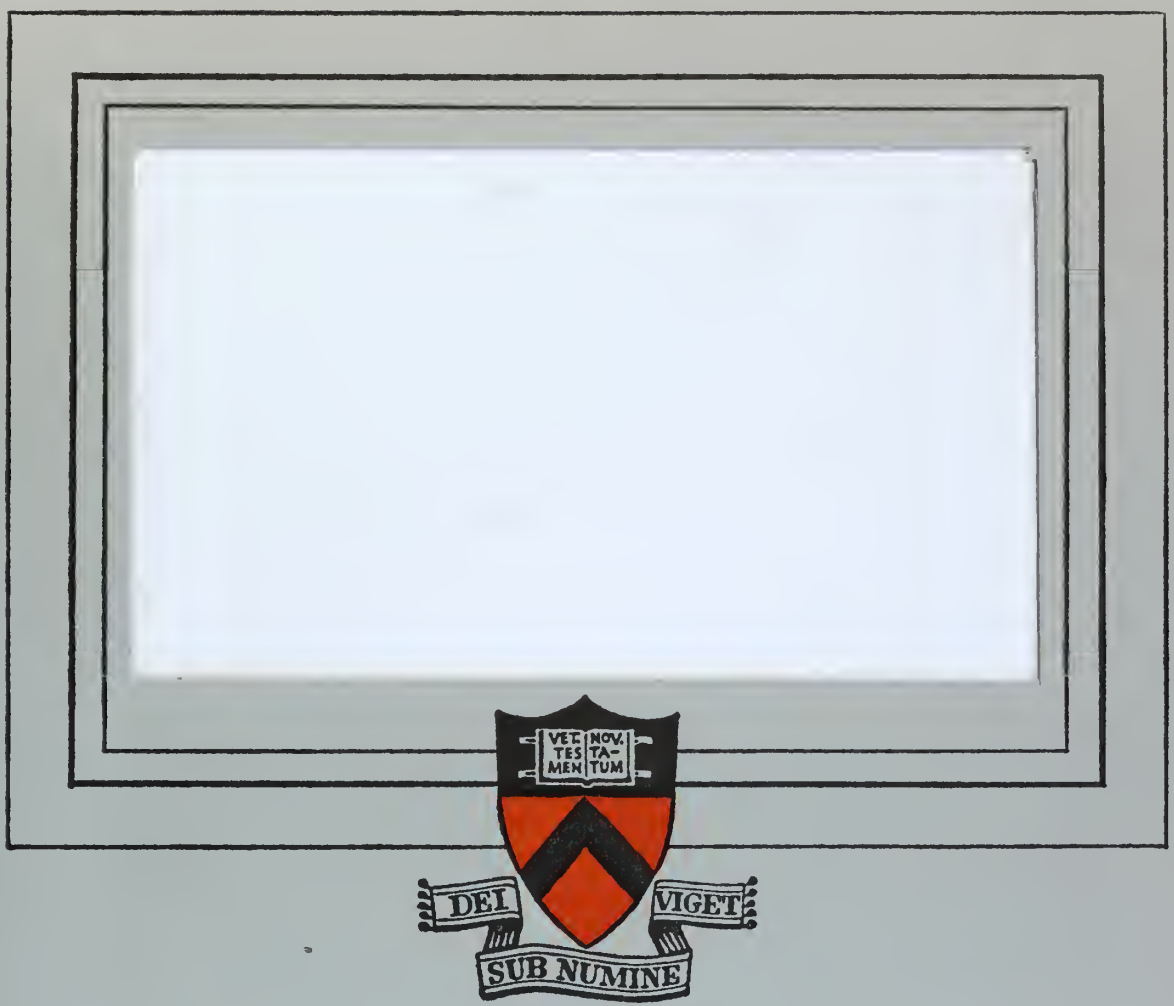
SENSITIVITY ANALYSIS OF A MULTI-PARAMETER PERFORMANCE FUNCTION AND APPLICATION TO A NUCLEAR ROCKET ENGINE SYSTEM

by

Robert J. Logan



The Aerospace Systems Laboratory

PRINCETON UNIVERSITY

DEPARTMENT OF
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SUMMARY

The use of computers to optimize free parameters of a system has become relatively widespread in many areas of engineering. Parameter optimization codes have been written for that purpose, and make it possible for a design engineer, once he has developed the mathematics of a system, to optimize its parameters according to some criteria. But of equal interest to the design engineer is the sensitivity of the optimized criteria to departure of the parameters away from their optimal value. The purpose of this thesis is to show ways in which a parameter optimization code may be augmented to yield such sensitivity information.

A Fletcher and Powell version of Davidon's variable metric optimization search technique was employed to optimize multi-parameter functions. Their method is useful in that it computes the inverse Hessian matrix (or matrix of second derivatives), which completely describes the curvature of the function at the optimum. Equations were developed so that the sensitivity could be expressed in a meaningful output format. This was made possible through the use of matrix inversion and eigenvalue analysis subroutines which were obtained from the scientific subroutine library of the IBM 360 91 and used in conjunction with a digital computer code employing the Fletcher and Powell technique. Equality constrained optimization problems were also considered by employing the penalty factor method proposed by Courant and used by Kelley. Equations analogous to the use of Lagrangian Multipliers were used to determine the cost of the equality constraint.

Example problems are offered showing the optimal solutions, sensitivity data at the optimum, and interpretation of that data. The well known Rosenbrock function was used to exhibit the accuracy of the methods employed. A typical engineering problem was solved involving the sensitivity of an optimal nuclear rocket engine used to inject a payload onto an interplanetary trajectory. The results indicated that the thermal power of the reactor and the ratio of length to diameter of the core could be varied considerably from their optimal values with little cost. The power density however was relatively fixed for optimal operation.

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LIST OF SYMBOLS

Sensitivity Analysis

a_{ij}	Element of Hessian matrix
F	Performance function to be minimized
F_x	First derivative of F with respect to X
G	Equality constraint on X variables
H	Hessian matrix of second derivatives at the optimum
k_i	Length of eigenvector
V_i	Normalized eigenvector of Hessian matrix
X	Vector of independent variables
Y	Dependent variable
ΔY	Allowable deviation in performance function
α	Step size parameter
Δ	Incremental change in variable
ε	Constraint violation
λ	Cost of constraint G
λ_i	Eigenvalues of Hessian matrix

Nuclear Rocket

D	Diameter of core
F	Total engine thrust
H_o	Initial orbital altitude
K_T	Tankage to propellant mass ratio
L	Length of core
$\dot{m}$	Total engine propellant mass flow

m_E	Total engine mass
m_o	Initial mass in earth orbit
NAR	Nozzle area ratio
p_c°	Nozzle chamber stagnation pressure
Q	Thermal power of reactor
$T_{c\ max}$	Maximum allowable core material temperature
V_{hf}	Final hyperbolic excess velocity
ψ	Power density of engine core

I. INTRODUCTION

The use of computers to optimize free parameters of a system has become relatively widespread in many areas of engineering. Parameter optimization codes have been written for that purpose, and make it possible for a design engineer, once he has developed the mathematics of a system, to optimize its parameters according to some criteria. But of equal interest to the design engineer is the sensitivity of the optimized criteria to departure of the parameters away from their optimal value. The purpose of this thesis is to show ways in which a parameter optimization code may be augmented to yield such sensitivity information. The interest in this is evident.

Since the engineer is working with temperatures, pressures, masses, etc., the computed optimal solution cannot be implemented exactly. Physical parameters are subject to uncontrollable variations and the resulting departure from the optimum may be quite significant. For space flight applications, maximum payloads might be of primary interest for one mission while a minimum fuel consumption the criterion for the next. Design requirements for a Venus flyby will certainly differ from those of a Mars lander or Jupiter probe, and yet many of the systems must be flexible enough to be useful for all three. Thus, the optimized solution must also contain significant information about departures from the optimum. This thesis addresses that problem; i.e. sensitivity analysis at the optimum.

Parameter optimization algorithms are many in number and varied in application. They differ primarily in their rate of convergence and the restrictions imposed on the function under consideration. Nearly all require a large number of iterations to achieve a given accuracy in locating

the optimum, and some procedures may not converge from a poor starting point.

Because, near the optimum, the second order terms in the Taylor series expansion dominate, the only method which will converge quickly for a general function are those which will guarantee to find the optimum of a general quadratic function speedily. Fletcher and Powell [1]* have produced such a method which was based upon a procedure described by Davidon [2]. The method is superior to other techniques which possess quadratic convergence in that it makes use of information determined by previous iterations and also in that each iteration is quick and simple to carry out. The primary justification for its use however, lies in the fact that the method yields the necessary information to determine the curvature of the objective function at the optimum.

The method of Fletcher and Powell estimates and continually updates the inverse of the Hessian matrix, H, (or matrix of second derivatives) during the optimization search so that a close approximation to the true value at the optimum is reached. Through the use of the eigenvalues and eigenvectors of the Hessian matrix, analysis of the characteristics of the objective function in the neighborhood of the optimum is possible.

As previously mentioned, it is of interest to know not only where the optimum is located, but by how much each parameter X_i may be changed from

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* Figures in parenthesis indicate references listed following the text.

its optimal value before a significant change, Δ, in the objective function occurs. The variation of the x_i may be independent of the other x_i, or several parameters may be changed simultaneously in a co-ordinated fashion away from the optimum. The latter variation might allow for significantly large departures from the optimum for a specified Δ when the function possesses the characteristics of an N-dimensional "ridge".

In this respect, it is intended that this thesis may be used to evaluate and analyze the optimum of any general function of N independent variables in such a way that a complete sensitivity at the optimum is clearly presented in a useful output format. It is shown to the user which of the specified variables may be changed and the magnitudes of those changes before specified degration in the objective function will be exceeded.

II. PROBLEM DEFINITION

An analysis of the behavior at the optimum of an N-variable function is possible where the second derivatives are known. Suppose that Y is a real valued function of N variables with continuous first and second partials and possesses a relative minimum at X_o, then the first derivative will vanish and by Taylor series expansion:

$$Y - Y_{opt} = \Delta Y = \frac{1}{2} \Delta X_o \left[\frac{\partial^2 y}{\partial x^2}\right] \Delta X_o + \text{Higher Order Terms} \tag{1}$$

where $\left[\frac{\partial^2 y}{\partial x^2}\right]$ is the Hessian matrix (H) of Y at the optimum.

From the Taylor series approximation (1) we find that the gradient

$$\Delta Y(X) = \left[\frac{\partial^2 y}{\partial x^2}(X)\right]^{-1} \nabla Y(X) \tag{2}$$

and solving for X_o yields:

$$X_o = X - \left[\frac{\partial^2 y}{\partial x^2}(X)\right]^{-1} \nabla Y(X) \tag{3}$$

so that if $\left[\frac{\partial^2 y}{\partial x^2}(X)\right]^{-1}$ were known, the step to the optimum would be given by (3). Some optimization algorithms collect information which

generate an approximation to the inverse Hessian matrix during the search for the optimum. These algorithms provide H^{-1} so that the problem of obtaining H, in the use of such an algorithm is reduced to the relatively simple additional task of inverting the N x N matrix $\left[\frac{\partial^2 y}{\partial x^2}\right]^{-1}$

Historically the method is similar to Newton's method which minimizes a function Y(x), x on N-vector, by generating a sequence of points (compare with equation (3))

$$X^{(k+1)} = X^{(k)} - \alpha^{(k)} \left[H^{(k)}\right]^{-1} \nabla Y^{(k)}$$

where $\alpha^{(k)}$ is an appropriately chosen scaler constant. Fletcher and Powell's version is in fact a quasi-Newton method which uses an initial estimate and computational history to generate an estimate to $\left[H^{(k)}\right]^{-1}$ rather than performing the computational work of evaluating and inverting the matrix at each step.

III. DAVIDON'S METHOD

Davidon introduced a variable metric method which was the first optimization technique to use past information estimating the inverse Hessian matrix. Fletcher and Powell have improved upon the method by simplifying the iteration scheme and modifying the criterion for convergence. Their method, which numerically determines the minimum of a function of several variables, combines the best features of the conventional gradient method and Newton's method, namely the sureness of convergence of the former and the quadratic terminal convergence of the latter. An excellent exposition of the method, including convergence proofs, has been given by Fletcher and Powell. For the purpose of this thesis however, it will suffice here to state the algorithm and point out the usefulness of its main features as was done by Kelley [3].

Let us denote the free parameters as X_i and the function to be minimized as $Y(x)$. It is assumed that Y has continuous first and second partial derivatives with respect to X. Any starting point X^o is chosen according to some criteria*. At the starting point X^o, the gradient vector Y_x as well as Y itself, is evaluated. A change is then made in X^o according to:

$$\Delta X = -\alpha H^{-1} Y_x \tag{4}$$

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* The freedom in the choice of the starting point depends on Y. If Y is well behaved, this choice is free. In other cases, the starting point must be close to the optimum to assure convergence.

where H^{-1} is a positive definite, symmetric matrix, defining a metric in the X-hyperspace. Its initial selection is otherwise arbitrary. For general purposes the unit matrix may be used, but if the parameters differ by orders of magnitude it is convenient to either scale them or to estimate the accuracy with which they are to be determined. $\alpha > 0$ is a step size parameter.

In Davidon's method, the one-dimensional minimum of F vs. α is obtained along the vector originating in X^o in the direction $H^{-1} Y_x$. At the new X, the gradient vector Y_x is again evaluated. The H^{-1} matrix is updated according to

$$H^{-1} + \Delta H^{-1} = H^{-1} + A + B \tag{5}$$

where

$$A = \frac{\Delta X \ \Delta X^{\top}}{\Delta X \ \Delta Y_x}$$

and generates the inverse of H in N steps for the quadratic function and where

$$B = - \frac{H^{-1} \Delta Y_x \Delta Y_x^{\top} H^{-1}}{\Delta Y_x^{\top} H^{-1} \Delta Y_x}$$

is intended to cancel the initial assumption for H_o^{-1} [4]. The procedure is begun again with the new values of X, Y_x, H^{-1}.

It is shown in [1] that H remains positive definite and that, as X approaches the minimizing point, H^{-1} approaches Y_{xx}^{-1} evaluated at the minimum. For quadratic Y, in N-dimensional space, the minimum is obtained in, at most, N steps (within round-off error): the method is quadratically convergent.

For more general functions having the smoothness properties assumed, a Taylor expansion through quadratic terms provides a good representation of the function in some neighborhood of the minimum. With H^{-1} converged, the minimum of Y vs. α then will occur for $\alpha = 1$,

$$\Delta X = -\alpha H^{-1} Y_x$$

will approach the value given by Newton's method, namely $-Y_{xx}^{-1} Y_x$.

IV. SENSITIVITY OF THE PERFORMANCE FUNCTION AT THE OPTIMUM

Assuming that the optimum and H^{-1} at the optimum have been determined and that H^{-1} has been inverted, then all the necessary information has been collected for a detailed analysis of the sensitivity of the performance function to changes in the performance parameters.

Let the criterion function be

$$Y(x_1, x_2, \ldots\ldots, x_n)$$

and assume for simplicity that the origin, i.e.

$$x_1 = x_2 = \ldots\ldots = x_n = 0$$

is an analytic optimum of Y. Around the optimum

$$Y = \frac{1}{2} X^T H X \tag{6}$$

where

$$H = \left| \frac{\partial^2 y}{\partial x_i \, \partial x_j} \right| = |a_{ij}|$$

is the Hessian matrix of Y at 0.

Independent Variation (one at a time)

If one parameter at a time is allowed to depart from the optimum, the function Y is

$$Y = \frac{1}{2} a_{ii} x_i^2$$

where a_{ii} is the corresponding diagonal term of H. For an assigned change Δ in Y we find

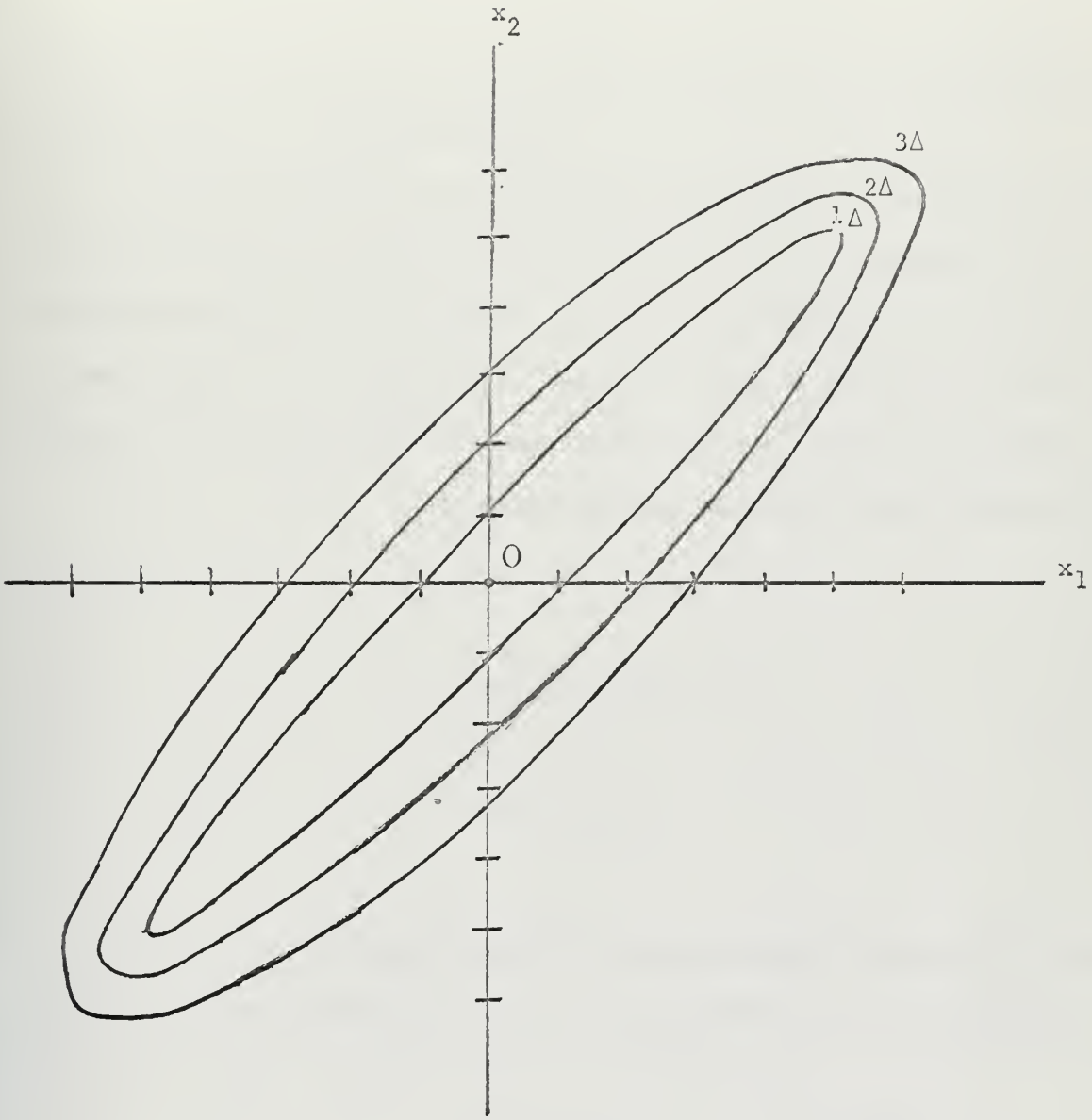
$$\pm \Delta x_i = \pm \sqrt{\left|\frac{2\Delta Y}{a_{ii}}\right|} \qquad (7)$$

where $\pm \Delta x_i$ is the allowable change in x_i for the previously assigned acceptable variation in Y.

Simultaneous Variation

If one allows several parameters to be changed in a co-ordinated fashion away from the optimum, departures from 0 for a specified ΔY may be significantly larger than those shown in the one-parameter-at-a-time case To illustrate this, consider the case in a 2-dimensional parametric space where the function Y presents the characteristics of a ridge as illustrated in Figure 1.

The $Y = 1\Delta$ line intersects the x_1 and x_2 axes at distances which are far less than the values of x_1 and x_2 at the end of the $Y = 1\Delta$ contour. (Five times less in the case of Figure 1).



A Skew Ridge Illustrating Advantage of Simultaneous Variation

Figure 1

Eigenvalues and Eigenvectors of H

To be able to analyze the characteristics of the Y surface in the neighborhood of 0, it is convenient to make use of the eigenvalues and eigenvectors of H at that point.

It is assumed here that the final use of this analysis will be in computer programs, and that matrices eigenvalue and eigenvector search subroutines are either available or easily implementable. To that respect, we note that H is a symmetric, positive definite matrix, and that knowledge of this fact simplifies the implementation of such subroutines.

Let λ_i and $\overline{V}_i$ be respectively the eigenvalues and eigenvectors of H [5], i.e.

$$\det (H - \lambda I) = 0$$

$$H \overline{V}_i = \lambda_i \overline{V}_i$$

Since H is real and symmetric the eigenvalues are real and the eigenvectors are orthogonal and may be expressed in orthonormal form:

$$\overline{V}_i^T \cdot \overline{V}_i = 1 \qquad \text{(normal)}$$

$$\overline{V}_i^T \cdot \overline{V}_j = 0 \quad i \neq j \quad \text{(orthogonal)}$$

If the N-parameters are allowed to be changed in the direction of the i^{th} eigenvector, i.e. $\overline{\Delta X} = k_i \overline{V}_i$, then the degradation in the performance function ΔY is:

$$\Delta Y = \frac{1}{2} k_i \bar{V}_i^T H k_i \bar{V}_i \tag{8}$$

but

$$H \bar{V}_i = \lambda_i \bar{V}_i \quad \text{and} \quad \bar{V}_i^T \cdot \bar{V}_i = 1$$

so that

$$\Delta Y = \frac{1}{2} k_i^2 \lambda_i \tag{9}$$

and for an allowable variation Δ in Y

$$k_i = \sqrt{\frac{2\Delta Y}{\lambda_i}} \tag{10}$$

k_i represents how far in the direction of the normalized i^{th} eigenvector one may travel on the response surface before degrading the performance function by ΔY. It is observed that k is a maximum for λ_{min},

so that the direction of least sensitivity to changes in the parameters, x_j is given by the eigenvector with $\lambda = \lambda_{min}$.

In other words the length of the $\bar{\Delta X}$ vector $= \sqrt{\sum_{j=1}^{N} \Delta X_j^2}$ is maximized for a given ΔY in the performance function.

Consider a hypothetical 2-variable optimization problem where the eigenvalues of H at 0 assume the values of 1 and 10, i.e.

$$\lambda_1 = 1; \quad \lambda_2 = 10$$

and the associated orthonormal eigenvectors are:

$$\bar{V}_1 = (1,0) \quad \text{and} \quad \bar{V}_2 = (0,1)$$

respectively. The contour of the objective function at the optimum will then assume the shape of Figure 2.

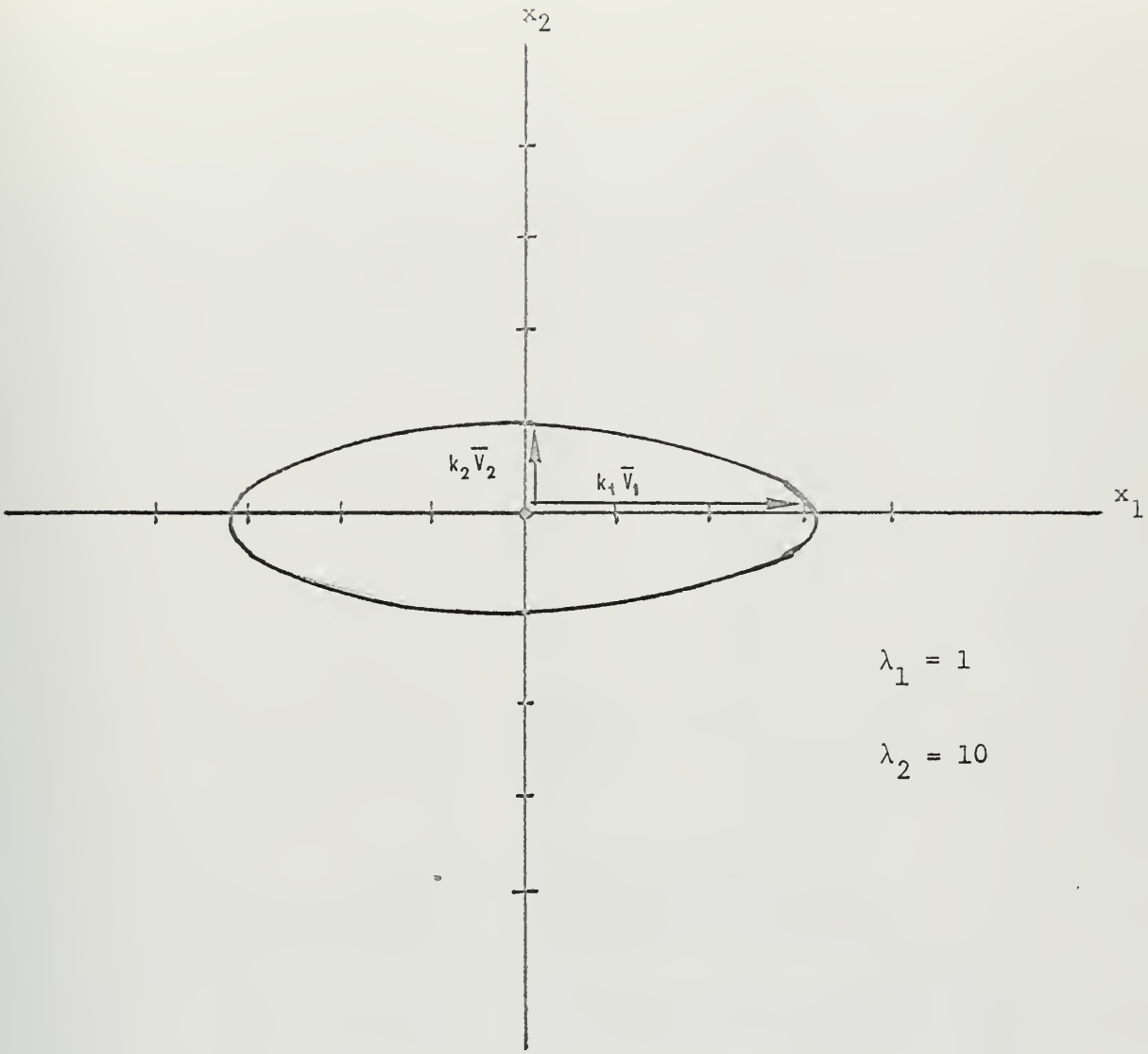
Observe that for a given Δy, the distance from the optimum in the direction of $\bar{V}_1$ is considerably greater than in the direction of $\bar{V}_2$. In fact, it follows directly from (10) that the distance is $\sqrt{\frac{\lambda_2}{\lambda_1}}$ greater. It is evident that the relative length of any existing ridges in the response surface will be determined by the square root of the ratio of any two eigenvalues and that the magnitude of the sensitivity for a given Δ will be determined by the square root of the eigenvalues.

Let two distinct solutions of optimization problems assume the values:

Solution 1 (as before)	Solution 2
$\lambda_{11} = 1 \quad \lambda_{12} = 10$	$\lambda_{21} = 0.1 \quad \lambda_{22} = 1$
$\bar{V}_1 = (1,0) \quad \bar{V}_2 = (0,1)$	$\bar{V}_1 = (1,0) \quad \bar{V}_2 = (0,1)$

The response surfaces will then assume the shapes of Figure 3a and Figure 3b respectively.

Notice that the ratio of the eigenvalues has remained constant and that the shape of the response surface is unchanged. The magnitude of the eigenvalues was decreased by a factor of 10 and if drawn to scale the response surface would be expanded in all directions by a factor of $\sqrt{10}$.



Effect of Eigenvalue Ratio on Response Surface

Figure 2

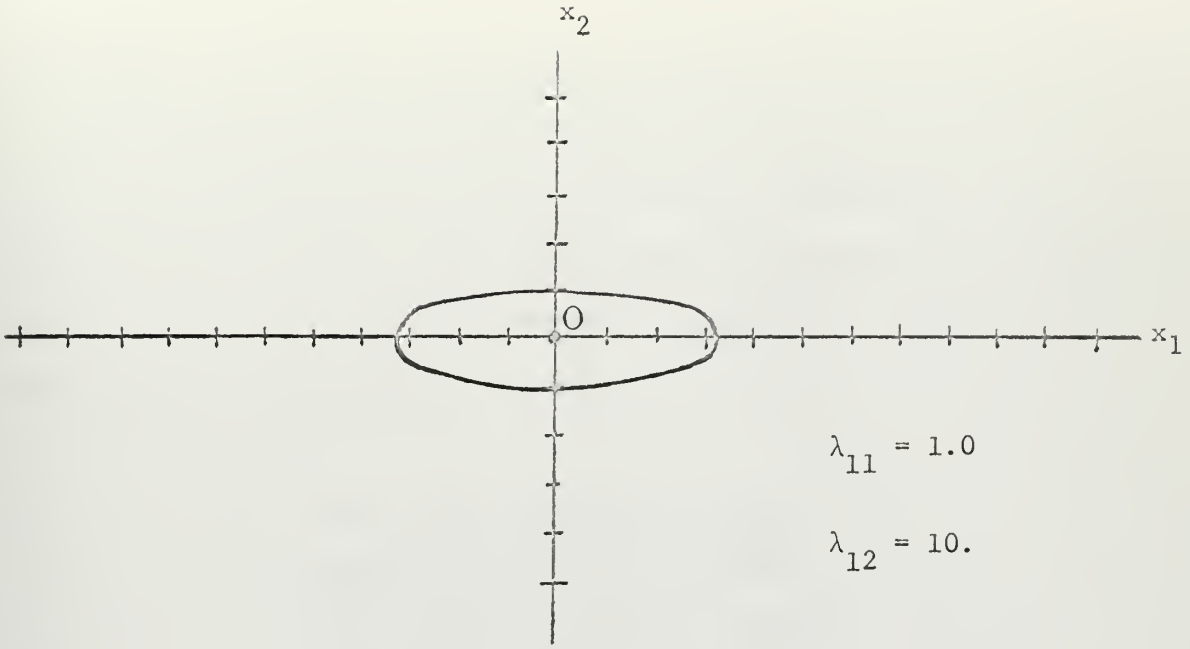


Figure 3a

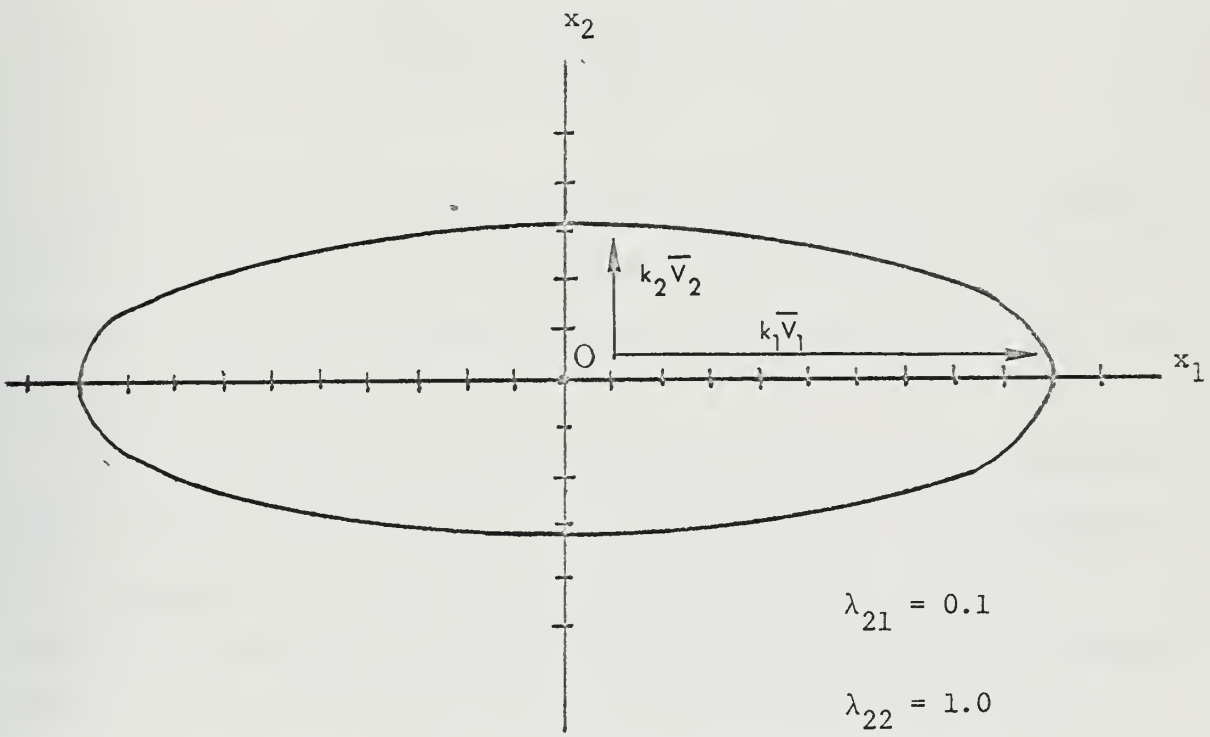


Figure 3b

Effect of the Magnitude of Eigenvalues on the Shape of the Response Surface

Figure 3

Skew Ridges

The previous examples have pointed out that when the matrix H has one eigenvalue much smaller than all other ones a ridge will exist in the response surface. A skew ridge exists when one eigenvalue is much smaller than all other ones, and the corresponding eigenvector is not parallel to one of the axis in X-space.

> If a ridge is parallel to one axis in X-space, it can always be removed by a change in scale along that axis. It is therefore representative of the way scales are chosen rather than a characteristic of the function to be optimized.

The situation is completely different if the ridge is at an angle to the axis because no change in scaling can remove the ridge. Such a ridge reflects an interaction between parameters in the way in which they affect the criterion function.

Only when the eigenvalues and eigenvectors of the Hessian matrix are known, can such a ridge be discovered; and only then can the characteristics of the optimum be determined. The complete search of eigenvalues and eigenvectors of H and the derivation of the resulting sensitivity information is contained in the computer program described in the following section.

V. COMPUTER PROGRAM

The program described in this thesis makes use of a standard, Powell-Fletcher type, parameter-optimization computer software package (6). It contains a multi-dimensional optimization algorithm similar to Davidon's variable metric method as was previously described.

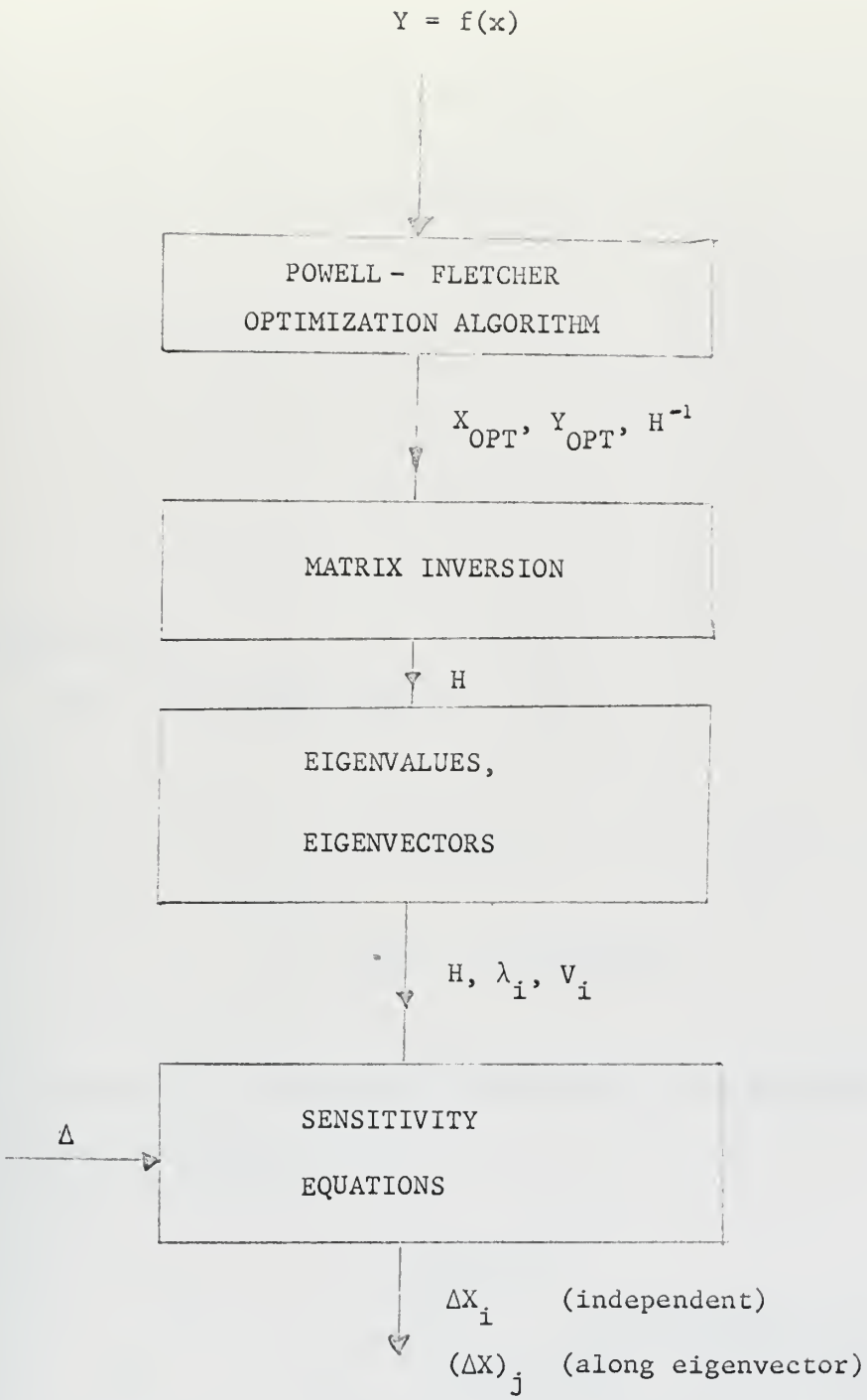
The matrix inversion and eigenvalue analysis subroutines were obtained from the scientific subroutine library of the IBM 360 model 91. A listing of these subroutines is presented in the Appendix. A simplified flow diagram illustrating the coordinated use of these programs is shown on the following page.

Necessary Input for Sensitivity Output

The input is the expression relating the objective function Y to the N independent variables x_i. The expression may take the form of a single equation, e.g.

$$Y = f(x_i)$$

or may comprise any number of subroutines as long as the objective function Y and the N independent variables are defined. The allowable departure Δ from the optimum is also a required input and must be specified by the user. It may be expressed as a percentage change in Y, e.g.



Flow Chart of Computer Programs

$$\Delta Y = 1\% \ Y_{opt}$$

or $$Y = 99\% \ Y_{opt}$$

or as a fixed quantity, e.g.

$$\Delta Y = 10.$$

Output Format

Given the required input:

$$Y = f(x_i)$$

$$Y = \Delta \quad \text{(a constant)}$$

the sensitivity information is presented in the following table for convenience in analysis.

TABLE I

Y_{opt}	ΔY	$x_{i_{opt}}$	Δx for Specified Δy			
			Independent Variation	Simultaneous Variation $\lambda_{min} = —$	$\lambda = ...$	$\lambda_{max} = —$
——	——	x_1	$\pm\Delta x_1$	Δx_1	...	Δx_1
		x_2	$\pm\Delta x_2$	Δx_2	...	Δx_2
		|	|	|	|	|
		|	|	|	|	|
		x_N	$\pm\Delta x_N$	Δx_N	|	Δx_N

VI. NUMERICAL EXAMPLE: ROSENBROCK FUNCTION

In order to illustrate the usefulness and accuracy of sensitivity analysis a standard test function is offered as an example. The function

$$Y(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

was proposed by Rosenbrock and is interesting in that it possesses a steep-sided ridge following the curve $x_1^2 = x_2$ as shown in Figure 4.

The exact solution of the problem is offered along with the computed values so that a comparison can be made and the effectiveness of the techniques employed may be evaluated.

Problem: minimize $Y = 100(x_2 - x_1^2)^2 + (1.0 - x_1)^2$

Exact Solution:

$$Y_{opt} = 0.0$$

$$x_1 = 1.0 \qquad H = \begin{vmatrix} 802 & -400 \\ -400 & 200 \end{vmatrix} \qquad H^{-1} = \begin{vmatrix} 0.5 & 1.0 \\ 1.0 & 2.005 \end{vmatrix}$$

$$x_2 = 1.0$$

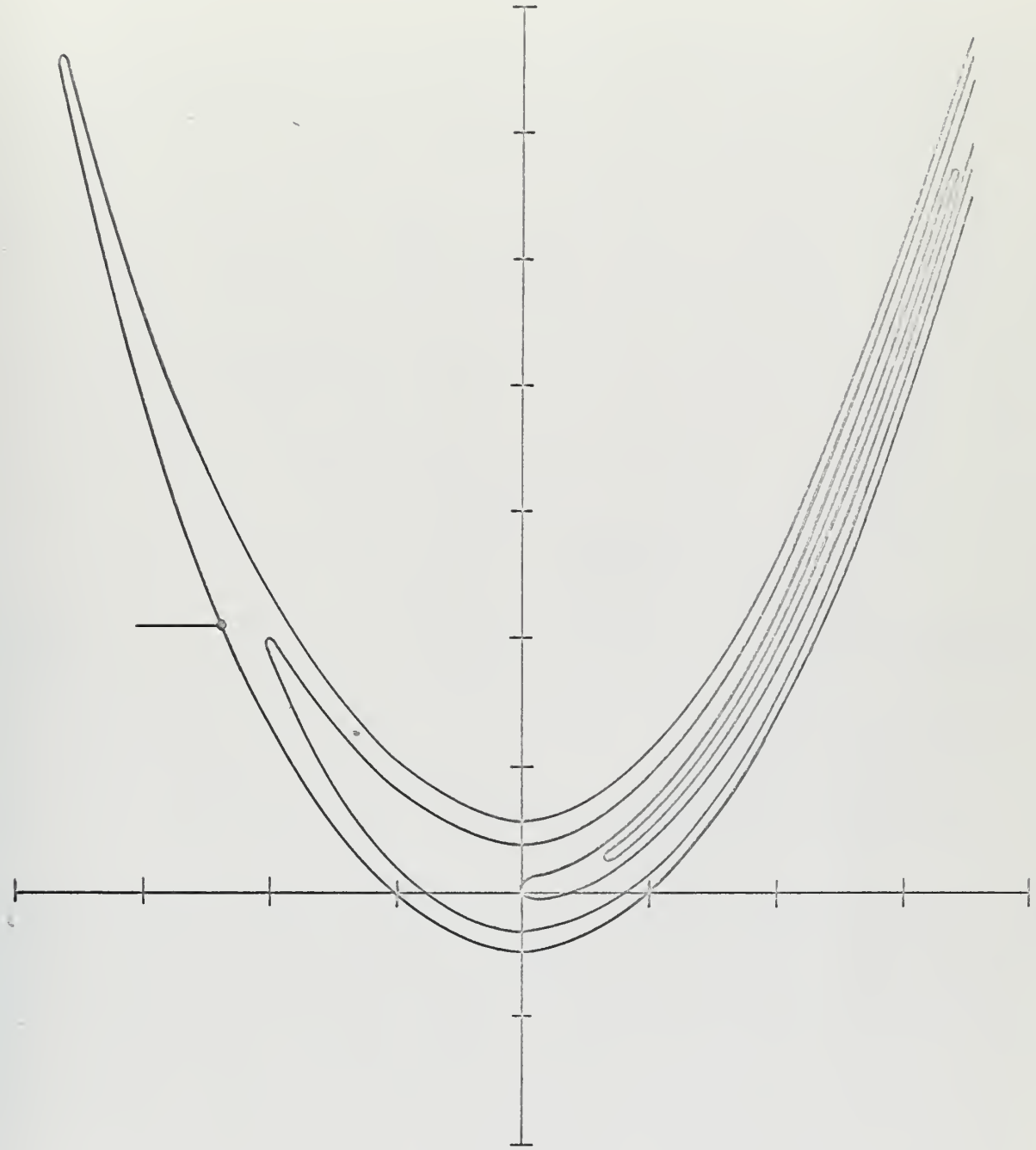
where all numbers given are exact.

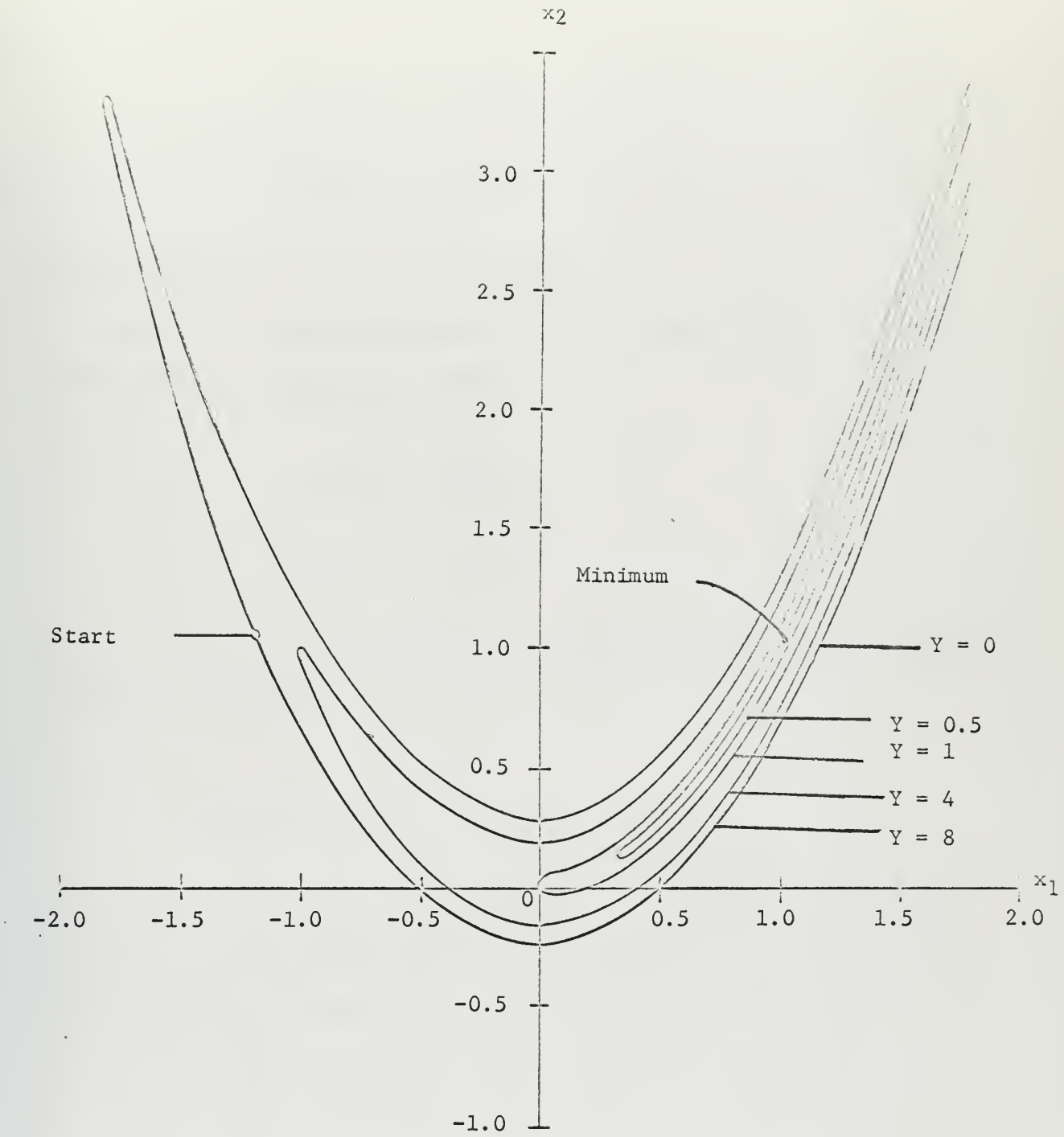
Fletcher and Powell's version of Davidon's variable metric technique found an optimum solution:

$$Y_{opt} = 10^{-6} \simeq 0.0$$

$$x_1 = 1.00007 \simeq 1.0$$

$$x_2 = 1.00017 \simeq 1.0$$





Rosenbrock's Curved Valley Function

Figure 4

and the approximated inverse Hessian matrix

$$H^{-1} = \begin{vmatrix} 0.5055 & 1.0051 \\ 1.0051 & 2.0035 \end{vmatrix}$$

which represents an error of less than 1%.

The matrix inversion subroutine with the approximated H^{-1} as its input resulted in the Hessian matrix:

$$H = \begin{vmatrix} 828.3 & -415.5 \\ -415.5 & 209.0 \end{vmatrix}$$

in error of about 4%. This error is more than acceptable for the purposes of sensitivity analysis.

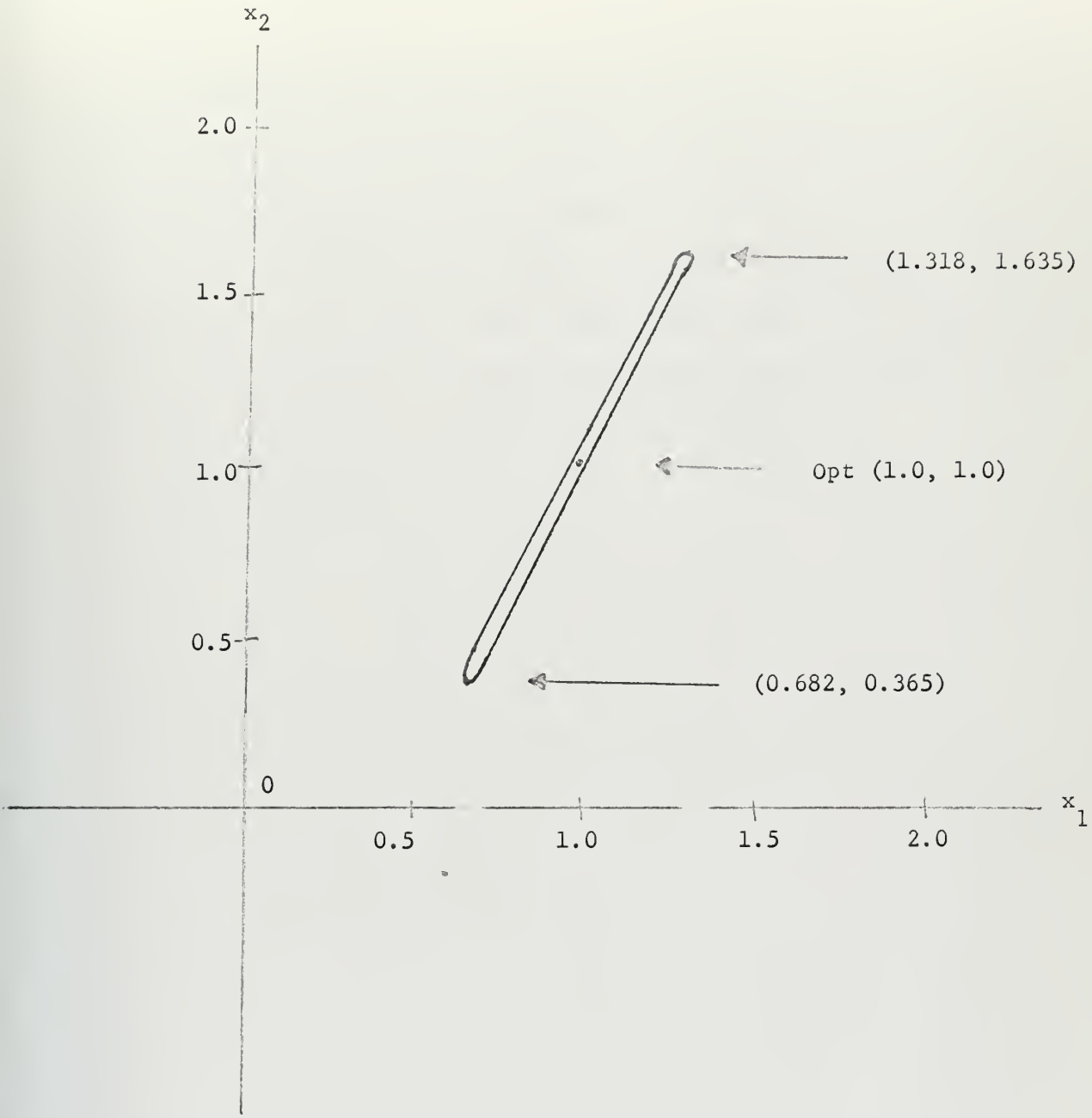
TABLE II

Sensitivity Data of Rosenbrock function:

Y_{opt}	ΔY	$x_{i_{opt}}$	Δx for Specified Δy		
			Independent Variation	Simultaneous Variation $\lambda_{min} = .399$	Simultaneous Variation $\lambda_2 = 1037.$
10^{-6}	0.10	1.00007	±.0155	$\Delta x_1 = +.319$	$\Delta x_1 = +.012$
		1.00017	±.0309	$\Delta x_2 = +.633$	$\Delta x_2 = -.006$

Analysis:

If the response surface were to be constructed from the sensitivity data shown with no knowledge of the function under consideration it would resemble Figure 5.



Predicted Shape of Rosenbrock Function at the Optimum

Figure 5

A comparison with Figure 4 shows that the sensitivity analysis at the optimum gives the desired results. The above figure shows that the function is extemely sensitive to changes along the x_1 axis ($\Delta x_1 = \pm .015$ for $Y = 0.1$) as well as to changes along the x_2 axis ($\Delta x_2 = \pm .031$). In contrast, it is shown that a skew ridge exists along the direction defined by $\Delta x_1 = .318$, $\Delta x_2 = .633$ and that if varied simultaneously x_1 may be changed by 30% and x_2 by 60% before Y changes by 0.1.

VII. EQUALITY CONSTRAINTS

In the optimization of multi-variable problems it is often the case that only certain combinations of the variables are either meaningful or acceptable. The imposed restriction usually assumes the form of an equality (or inequality) constraint:

$$G(x_i) = 0$$

The analytical solution of such a problem can be found by the method of Lagrangian Multipliers [7], which seeks values of the parameters for which the modified objective function

$$F^* = F + \lambda G \tag{11}$$

is stationary, i.e.

$$F_x^* = F_x + \lambda G_x = 0 \tag{12}$$

Solving for λ yields

$$\lambda = -\frac{F_x}{G_x} \tag{13}$$

λ is meaningful in that it represents the cost of the constraint G. If G were relaxed by 1 unit then F could vary by λ.

In the general case however, numerical search methods are unlikely to locate all types of stationary points for the modified function using Lagrangian Multipliers. A more feasible approach is that of penalty factors. [8]

Penalty Factors

In the use of penalty factors a modified function which incorporates the constraint is defined as

$$F^* = F + PG^2 \tag{14}$$

where P is a large positive-valued constant (for minimization). If P is chosen large enough then G is forced close to zero in the search for the optimum. At the optimal solution G is equal to some small quantity ε. If ε is not within an acceptable distance from G then P is increased until an optimum is found which satisfies G within ε. The cost of the constraint can be found in a manner identical to the method of Lagrangian Multipliers.

At the optimum of the modified function of (14)

$$F_x^* = F_x + 2P\varepsilon\, G_x = 0 \tag{15}$$

so that

$$2P\varepsilon = -\frac{F_x}{G_x} = \lambda \tag{16}$$

is the cost of the constaint G.

Although the idea of a penalty function seems to have been conceived some years ago (Courant [1943]), there has been very little computational experience with regard to its applications. By examining equation (16) it is observed that as ε approaches zero, P becomes infinitely large. Large values of P however effectively produce a sharp ridge in the contours of F^*, and most search techniques are troubled by the existence of such a ridge. The choice of P is therefore a compromise between large values for small violations in G, and smaller values to eliminate troublesome ridges in the modified objective function.

In using Davidon's optimization technique however, it was discovered that even if a ridge presents no problem in finding the optimal solution, P may <u>not</u> be chosen arbitrarily large. For this situation, ε becomes so small that changes in the parameters of order ε produce corresponding changes in F which are less than the criterion for convergence in the search for the optimum. If ε is to be meaningful it must be large enough to possess a unique solution. In other words changes in ε must be large enough to affect the terminal convergence of the optimization search. It is therefore necessary to possess some insight into the problem before the penalty factor method can be employed.

We may note that for any given equality-constrained optimization problem, λ will possess a unique value. Analytically λ is found to be $2P\varepsilon$ as ε approaches zero and P approaches infinity. Let us denote ε_{max} as the maximum allowable violation in the equality constraint and ε_{min} as the minimum ε which will produce a unique optimum within the limits of the convergence criterion. ε must now satisfy

$$\varepsilon_{min} < \varepsilon < \varepsilon_{max}$$

for a meaningful solution.

Values for λ and P are estimated within one or two orders of magnitude such that

$$2P_{(est)}\ \varepsilon = \lambda_{(est)}.$$

If the resulting optimum possesses an allowable ε then the solution is found with the cost of the constraint

$$\lambda = 2P\varepsilon \tag{17}$$

and the constraint violation:

$$\varepsilon = G_{opt} - G \tag{18}$$

If $\varepsilon > \varepsilon_{max}$ or $\varepsilon < \varepsilon_{min}$, then P must be increased or decreased respectively until an allowable ε is found.

Example Problem

To illustrate the use of the penalty factor method for equality constrained optimization problems the following two examples are offered for comparison and analysis.

Let $F_1(x_1, x_2) = F_2(x_1, x_2) = (x_1 - 3)^2 + (x_2 - 3)^2$

and $G_1(x_1, x_2) = x_1 + x_2 - 4 = 0$

$G(x_1, x_2) = x_1 x_2 - 4 = 0$

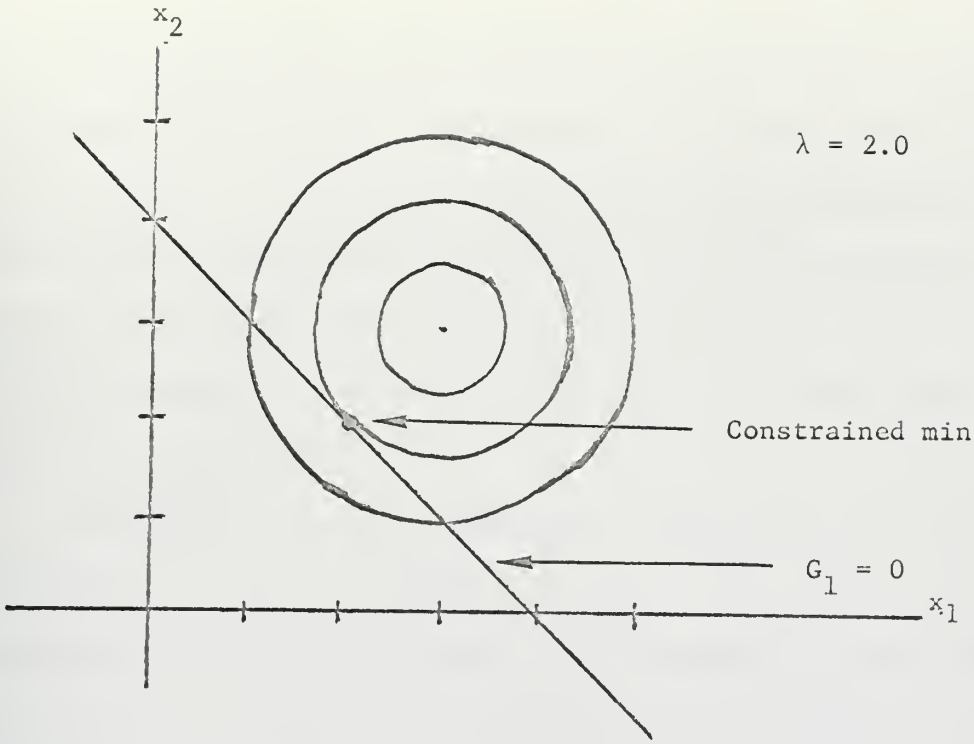


Figure 6a

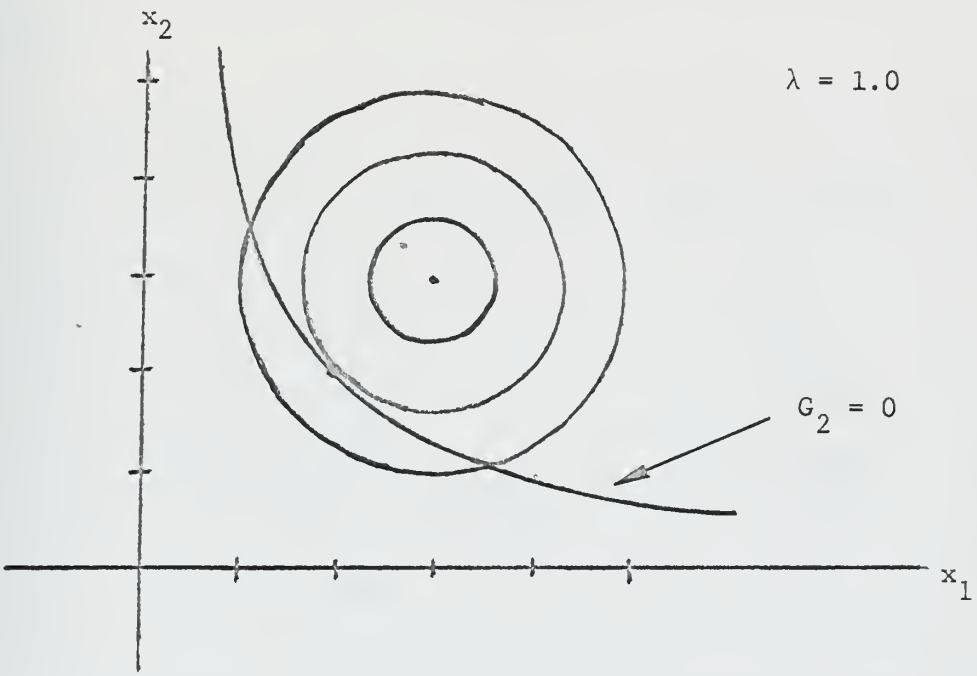


Figure 6b

Interpretation of Cost of the Constraint $\frac{-F_x}{G_x}$

Figure 6

The response surfaces are shown in Figure 6, where the equality constrained function has a minimum value at the same point for both problems, i.e. $x_1 = x_2 = 2.0$. Since the unrestricted function is the same and the solution lies at the same point, then the gradient F_x is the same for both problems. The constraint and its gradient G_x are different however and consequently the cost of the constraint λ will have two distinct values.

Analytically it can be shown that $-F_x/G_x = \lambda = 2$ for the linear constraint $x_1 + x_2 = 4$ and that $-F_x/G_x = \lambda = 1$ for the hyperbolic constraint $x_1 x_2 = 4$. The cost of the constraint has been reduced in the second case because F is less sensitive to changes in G_2 at the optimum.

Computer Results:

For $F^* = F + P\,G_1^2$	and	$F^* = F + P\,G_2^2$
and $P = 100$		$P = 100$
$F^* = 1.980$		$F^* = 1.994$
$x_1 = 2.005$		$x_1 = 2.0009$
$x_2 = 2.005$		$x_2 = 2.0020$
$\varepsilon = G^* - G = .010$		$\varepsilon = .0057$
$\lambda = 1.988$		$\lambda = 1.141$

In the second case, a minimum was found which was very close to the constraint, e.g. $\varepsilon = .0057$. As a result $\lambda = 1.141$, a difference of .141 from the analytical value. This error may be explained by examining the magnitude of ε. An ε of .0057 is very small for the problem under

consideration. Changes in the variables of order ε will not affect the optimal solution, so that ε is actually less than ε_{MIN} as previously defined.

A second optimization was performed with P reduced to 50 in order to increase ε. (Remember that it has been shown that $2P\varepsilon$ is constant). The results were:

$$F^* = 1.989$$

$$x_1 = 2.0065$$

$$x_2 = 1.999$$

$$\varepsilon = .011$$

$$\lambda = 1.07$$

It is observed that decreasing P resulted in a more meaningful value for ε and consequently a closer approximation to the const constraint, λ.

VIII. SENSITIVITY ANALYSIS OF A NUCLEAR ROCKET ENGINE

As was previously mentioned, the primary purpose of a sensitivity analysis is to aid the design engineer in constructing a system which will operate in an optimal fashion, despite variations in the controlling parameters. To that effect, an illustrative example is presented whereby the engine design parameters of a nuclear rocket are optimized in order to achieve a maximum payload at a specified hyperbolic velocity.

A set of mathematical models of the elements of nuclear rocket engines, suitable for detailed systems analysis, has been developed [9] which constitutes the basis for a digital computer program called NUROC/SAC (Nuclear Rocket Systems Analysis Code). The Code has been used to describe a number of existing engines and the results obtained were found to be accurate [10].

ESCAPE [11] is another computer code which calculates geocentric (or planetocentric) tangential thrust escape trajectories and which may be used in conjunction with NUROC/SAC.

Input Parameters

From a design viewpoint the most important input parameters to NUROC/SAC are:

Q	thermal power of the reactor, watts
D	diameter of the reactor core, meters
L	length of core, meters
L/D	ratio of core length to diameter
T_{cmax}	maximum allowable core material temperature, °K

p_c°	nozzle chamber stagnation pressure, n/cm^2
NAR	nozzle area ratio: A_{exit}/A_{throat}

The output format of NUROC/SAC consists of a summary of operating variables including the input design parameters, defining entirely the characteristics of a specific nuclear rocket engine. The most important of these and the ones which will be used as inputs into ESCAPE are:

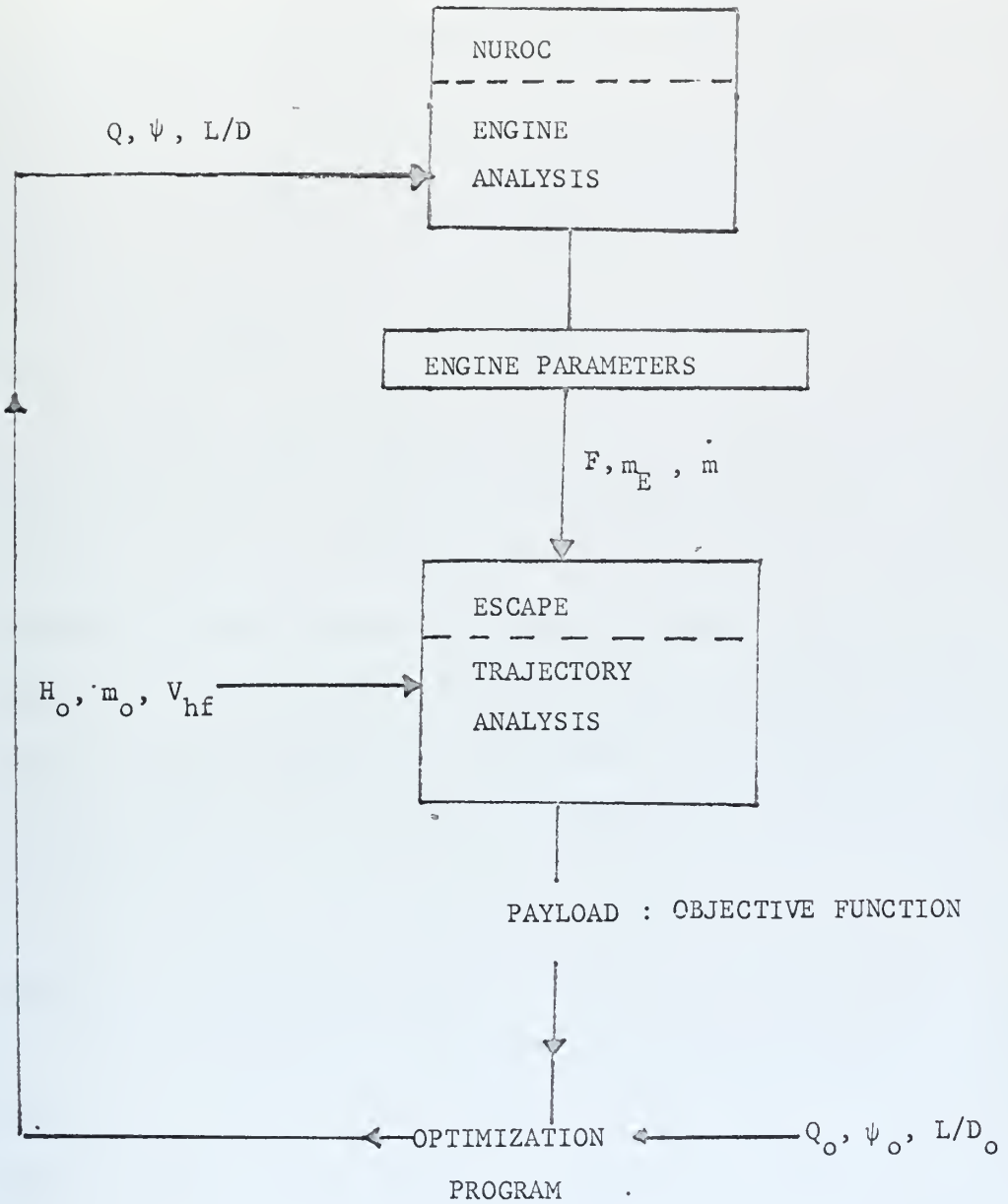
$\dot{m}$	total engine propellant mass flow
F	total engine thrust
m_E	total engine mass

Additional inputs to ESCAPE which must be specified are:

m_o	initial mass in earth orbit
H_o	initial orbital altitude
V_{hf}	final hyperbolic excess velocity specified
K_T	tankage to propellant mass ratio

The output of ESCAPE may assume a variety of formats but the payload delivered at the specified hyperbolic velocity is the payoff in the optimization problems which follow. The payload is defined as the initial mass minus the engine mass, the tankage mass, and the propellant mass required to reach V_{hf}.

A previous study [12] has indicated that within the range described by technological constraints the payload performance of the nuclear rocket will increase monotonically with the maximum allowable core material



Subroutines Used to Generate the Objective Function for Nuclear Rocket Optimization

temperature and the nozzle area ratio, and will decrease monotonically with the chamber stagnation pressure. Thus choice of these parameters is limited to technologically realizable values. Typical values presently in use are:

$$T_{cmax} = 3000\ ^{\circ}K$$

$$p_c^{\circ} = 300\ n/cm^2$$

$$NAR = 100.$$

The power, power density, diameter, and length which parameterize the core geometry may be varied in a constrained but optimal fashion to describe an engine which will inject the maximum payload into a specified interplanetary trajectory for a given initial mass in earth orbit. The problems which follow will consider an initial mass of 100,000 kilograms in an earth orbit of 500 kilometers and will optimize the core geometry to inject the maximum payload into a trajectory described by a hyperbolic excess velocity of 10,000 m/sec.

Optimization of Core Geometry

It is interesting to note that if any three of the four engine parameters, power (Q), power density (ψ), diameter (D) and length (L), are specified then the fourth is automatically determined. Since the length and diameter describe the volume, the power density can be expressed as a function of Q, L, D, i.e.,

$$\psi = 4Q/\pi D^2 L$$

Thus the optimization of core geometry is reduced to a 3-dimensional problem.

Maximize Payload: Free Parameters Q, ψ, L/D

The following example maximizes the payload delivered by a nuclear rocket with free parameters: power (Q), power density (ψ), and ratio of length to diameter (L/D).

Starting Point:

$$Q = x_1 = 2000.\ \text{MWt}$$
$$\psi = x_2 = 6.0 \times 10^9\ \text{W/m}^3$$
$$L/D = x_3 = 4.0$$

TABLE III

Sensitivity Data at the Optimum

Y_{opt}	$\Delta Y = 1\%$	X_{opt}	Δx for Specified Δy			
			Independent Variation	Simultaneous Variation $\lambda = 39.5$	$\lambda = 1105.$	$\lambda = 6150$
31,630 Kg.	316. Kg	Q=1832 MWt	$\Delta Q = \pm 333.$	68.	-28.	28.
		$\psi = 8.84 \times 10^9$ W/m^3	$\Delta\psi = \pm 3.03$ ($\times 10^9$)	3.88 ($\times 10^9$)	-.062 ($\times 10^9$)	-.017 ($\times 10^9$)
		L/D=4.80	$\Delta L/D = \pm .57$	.387	.677	.199

Analysis:

When both ψ and L/D are free parameters the optimized values become so high that the cost of the uranium necessary to make such a reactor critical would become prohibitively expensive. Also, a length to diameter ratio of approximately 5 and a power density of 9×10^9 W/m^3 would describe a highly inefficient reactor due to excessive neutron leakage through the core ends. Other important design factors (such as

shielding), which are not now contained in NUROC/SAC, indicate that the length should be only slightly larger than the diameter. It should also be noted in the sensitivity data that ψ is quite flexible ($\Delta\psi = \pm 3 \times 10^9$) and that smaller values may be chosen with little resulting loss in payload.

This problem should serve as an example that one cannot randomly optimize variables or undertake a sensitivity analysis without first acquiring a knowledge of the system under consideration. With these facts in mind, a second optimization problem is solved in two-dimensions with L/D fixed at 1.5.

Maximize Payload: Free Parameters Q, ψ

Starting Point:

$$Q = x_1 = 2000 \text{ MWt}$$

$$\psi = x_2 = 6.0 \times 10^9 \text{ W/m}^3$$

TABLE IV

Sensitivity Data at the Optimum

Y_{opt}	$\Delta Y = 1\%$	X_{opt}	Δx for Specified Δy		
			Independent Variation	Simultaneous Variation $\lambda = 5151$	Simultaneous Variation $\lambda = 23630$
30,938Kg.	309.	Q=1823 MWt	$\Delta Q = \pm 339.$	340.	9.6
		$\psi = 4.97 \times 10^9$ W/m^3	$\Delta\psi = \pm .160$ ($\times 10^9$)	$-.02$ ($\times 10^9$)	$.159$ ($\times 10^9$)

Analysis:

The restriction on L/D (fixed at 1.5) results in a loss in optimal payload of only 2 percent. It is interesting to note that the optimal power and allowable deviation are almost identical to the three-variable problem. The power density however has a considerably lower optimal

value and $\Delta\psi$ is much smaller when L/D is fixed.

The sensitivity data reveals that any power between 1500 and 2150 MWt may be used if ψ is held constant with only a small (1%) resulting loss in payload. In contrast the power density must remain close (within 4%) to 5.0×10^9 W/M^3. The fact that the eigenvectors are located close to the Q and ψ axes implies that little more can be gained by varying Q and ψ simultaneously.

Maximize Payload: Free Parameters Q, L/D

With the discovery that ψ and L/D cannot both be free and having fixed L/D at 1.5 it would now be advantageous to fix ψ and optimize on Q and L/D. A value of 3.0×10^9 W/M is chosen for the power density based on accepted values for existing nuclear rocket engines.

Starting Point:

$$Q = x_1 = 2000 \text{ MWt}$$

$$L/D = x_2 = 2.0$$

TABLE V

Sensitivity Data at the Optimum

Y_{opt}	$\Delta Y = 1\%$	X_{opt}	Δx for Specified Δy		
			Independent Variation	Simultaneous Variation $\lambda = 935.$	$\lambda = 3867.$
30,675 Kg.	306.	Q = 1542 MWt	$\Delta Q = \pm 397$	$\Delta Q = 114$	$\Delta Q = 390$
		L/D = 1.67	$\Delta L/D = \pm .78$	$\Delta L/D = 0.79$	$\Delta L/D = -.056$

Analysis:

When the power density is fixed both the power and the ratio of length to diameter have large acceptable variations. The power may vary from 1150

to 1950 with L/D and ψ fixed, and L/D may vary from 1.9 to 2.45 with Q and ψ fixed. This allows for considerable flexibility in designing an optimal engine as long as the power density remains relatively constant.

The least sensitive direction of change is associated with the minimum eigenvalue. The associated eigenvector indicates that L/D may still vary from .9 to 2.45 and Q need not remain fixed, but may vary by ±114 MWt as long as the direction of change from the optimal value coincides with changes in L/D.

Verification of Results

In order to verify that the predicted sensitivity of the optimized variables is accurate, the allowable deviations were substituted into NUROC/SAC and ESCAPE and the resulting payload was computed. A comparison was made to check if the payload remained within the predicted 1% of the maximum. The optimal values were first rounded-off to Q = 1550 ±400 MWt; L/D = 1.67 ±.75.

TABLE VI

Comparison:

Maximum payload minus 1% = 30,370 Kg.

Independent Variation		L/D	Payload (Kg)
I. ΔL/D, Q fixed		.90	30,271
		2.45	30,520
II. ΔQ, L/D fixed		Q	
		1150. MWt	30,295
		1950. MWt	30,420
Simultaneous Variation	Q	L/D	
	1435	.90	30,135
	1665	2.45	30,445

The table of comparisons indicates that if Q and L/D are increased either independently or simultaneously the loss in payload is even less than the predicted 1%. If decreased the deviations become slightly larger than 1% but are still highly accurate. This may not always be the case.

It must be realized that the sensitivity analysis is accurate only at the optimum. For functions which are very flat (i.e. insensitive to change) the predicted variations may be quite large, as indeed they are in the example given. When the variations are substituted, the function is no longer close to the optimum and results may vary considerably from those predicted. For this reason it is prudent to verify results especially at points far from the optimum.

Another reason for verifying results is that there exist small inherent errors in the optimization search, matrix inversion and eigen analysis subroutines. Care should also be taken in defining the convergence criterion because if the computer is forced to make repeated searches near the optimum the values for the inverse Hessian matrix will be destroyed. Any resulting sensitivity analysis will be meaningless.

Application of Penalty Factor

In the previous two-dimensional optimization problem an optimal power of 1550 MWt and length to diameter ratio of 1.67 was established for a fixed power density of 3.0×10^9 M/W^3. As was previously mentioned for equality constrained problems it is of interest to know the cost of the restriction on power density λ. The following example employed the penalty factor method to optimize a three-variable problem with the constraint:

$$G(x_3) = x_3 - 3.0 \times 10^9 = 0$$

Starting Point:

$$Q = x_1 = 2000 \text{ MWt}$$

$$L/D = x_2 = 6.0$$

$$\psi = x_3 = 4.0 \times 10^9 \text{ W/M}^3$$

$$\text{Penalty Factor} = P = 10{,}000$$

Results:

$$\text{Payload} = 30{,}670 \text{ Kg.}$$

$$Q = 1547 \text{ MWt.}$$

$$L/D = 1.7$$

$$\psi = 3.020 \times 10^9 \text{ W/M}^3$$

$$\varepsilon = G^* - G = .020$$

$$\lambda = 2P\varepsilon = 406.$$

The cost of keeping the power density constant is 406 Kg. of payload per (10^9 W/m^3).

IX. CONCLUSIONS AND RECOMMENDATIONS

A sensitivity analysis at the optimum has been performed through the use of existing computer codes. By simply defining an objective function and any number of independent variables an optimized solution is found. In addition, it has been shown that the sensitivity of each of the variables at the optimum may be given in a useful format. With all others held constant, the range that each variable may assume before a specified degradation in performance occurs is given. Also, the length and direction of the axis of all ridges in the objective function are listed in order of decreasing magnitude. With this information at hand a complete knowledge of the sensitivity of all the input parameters is available to the user and decisions regarding optimal parameter choice can be made, taking into account the flexibility given by the sensitivity knowledge.

The methods employed were shown to be highly accurate when dealing with purely mathematical problems. The sensitivities of Rosenbrock's parabolic valley function were found with little difficulty. Engineering applications, on the other hand, require a great deal of insight into the problem before a sensitivity analysis may be started. Scaling the variables is important so that the sensitivity information is meaningful. The nuclear rocket example studied the engine performance related to power, power density and ratio of length to diameter of the nuclear core. A scaling problem existed because the power in watts and power density in watts/cubic meter were of the order of magnitude of 10^9, while the length/diameter was approximately unity. Usually such a problem can be

avoided by normalizing each variable by dividing it by the order of magnitude. This would be fine if the acceptable deviations occurred within the same number of significant figures. However, if one variable is much less sensitive to change than all the others, then the eigenvector associated with the minimum eigenvalue will be dominated by that component and very little knowledge can be gained about the other variables in that direction. It would be convenient to modify the computer program so that the sensitivities would be normalized instead of the variables. Of course, the user could always eliminate the problem by normalizing the variables the first time, and after observing the resulting deviations, normalize the sensitivities and optimize again. The optimized solution will be the same but the sensitivity data will be more accurate and meaningful.

Another problem experienced when working with engineering problems was in defining a convergence criterion. For the Rosenbrock function a change in the variables of 10^{-4} produced significant changes in the objective function. When optimizing the nuclear rocker, however, the maximum payload was essentially determined when the normalized variables were accurate in the second decimal place. With the convergence criterion set at 10^{-4}, the program made over a hundred more iterations before stopping and found an optimum which was only about one kilogram more in payload. When the optimization search stays close to the optimum for many iterations, the inverse Hessian matrix is destroyed and any resulting sensitivity analysis has no meaning. A modification in the program is required so that when the optimum has essentially been determined, the inverse Hessian matrix can be stored and any subsequent refinement of the optimum will not affect the sensitivity data.

Equality constrained optimization has been discussed but not in detail. The penalty factor method used by Kelley was implemented to determine an approximation to what is usually referred to as the cost of the constraint.

It would also be of interest to know how far in the plane of the constraint and normal to it, one may travel on the response surface before reaching a specified change in the optimum. This thesis has not considered such a sensitivity analysis. The techniques involved are similar, but more attention is needed in this area.

Inequality constrained optimization problems are generally no more difficult to solve than equality constrained ones. For well behaved functions, the solution either does not violate the constraint or lies on the boundary and may be treated as an equality constraint. In either case, the techniques developed in this thesis can be applied. Care should be taken to try a variety of starting points so that if the same solution is reached, the function can be assumed to be well behaved.

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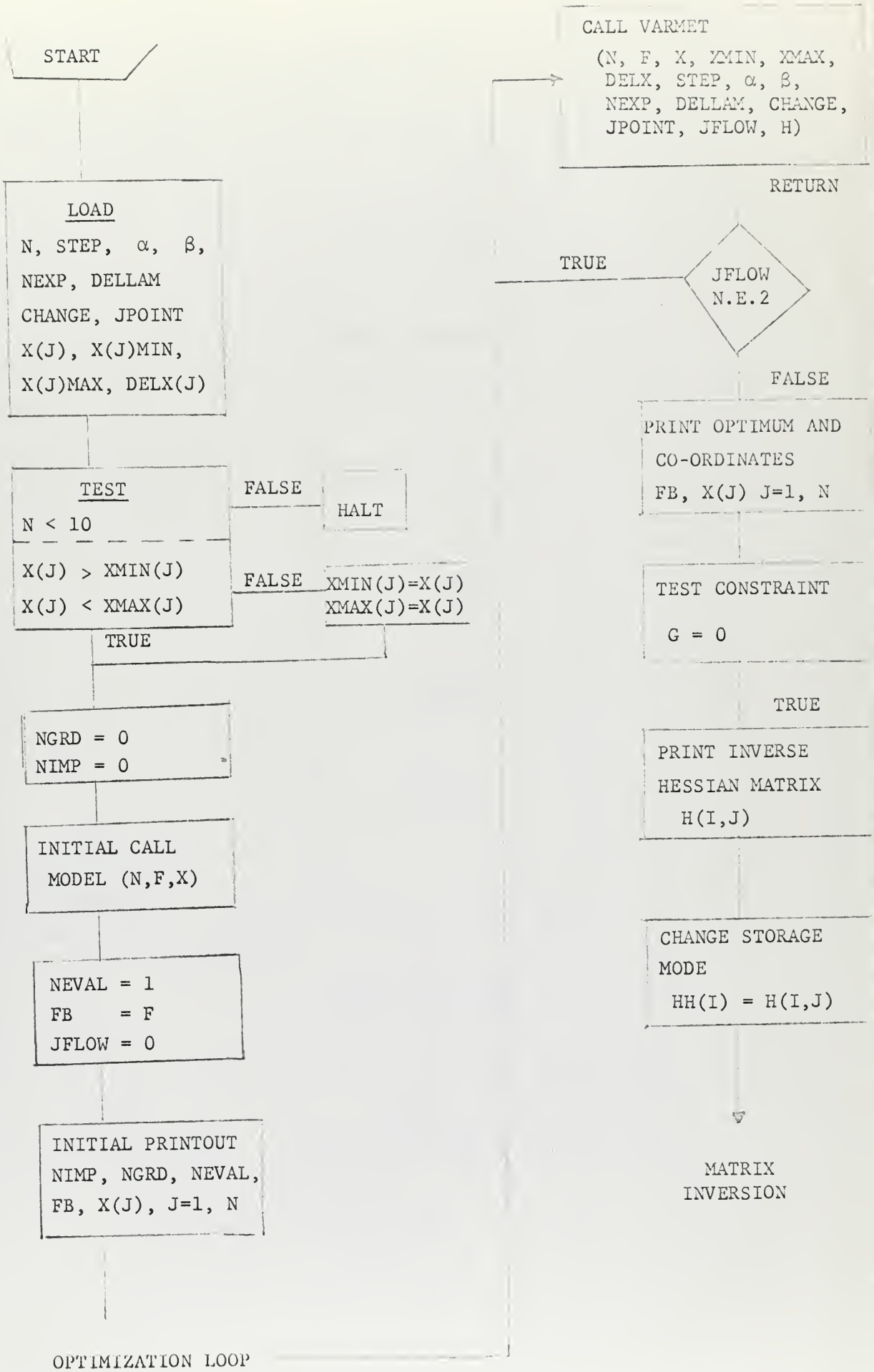
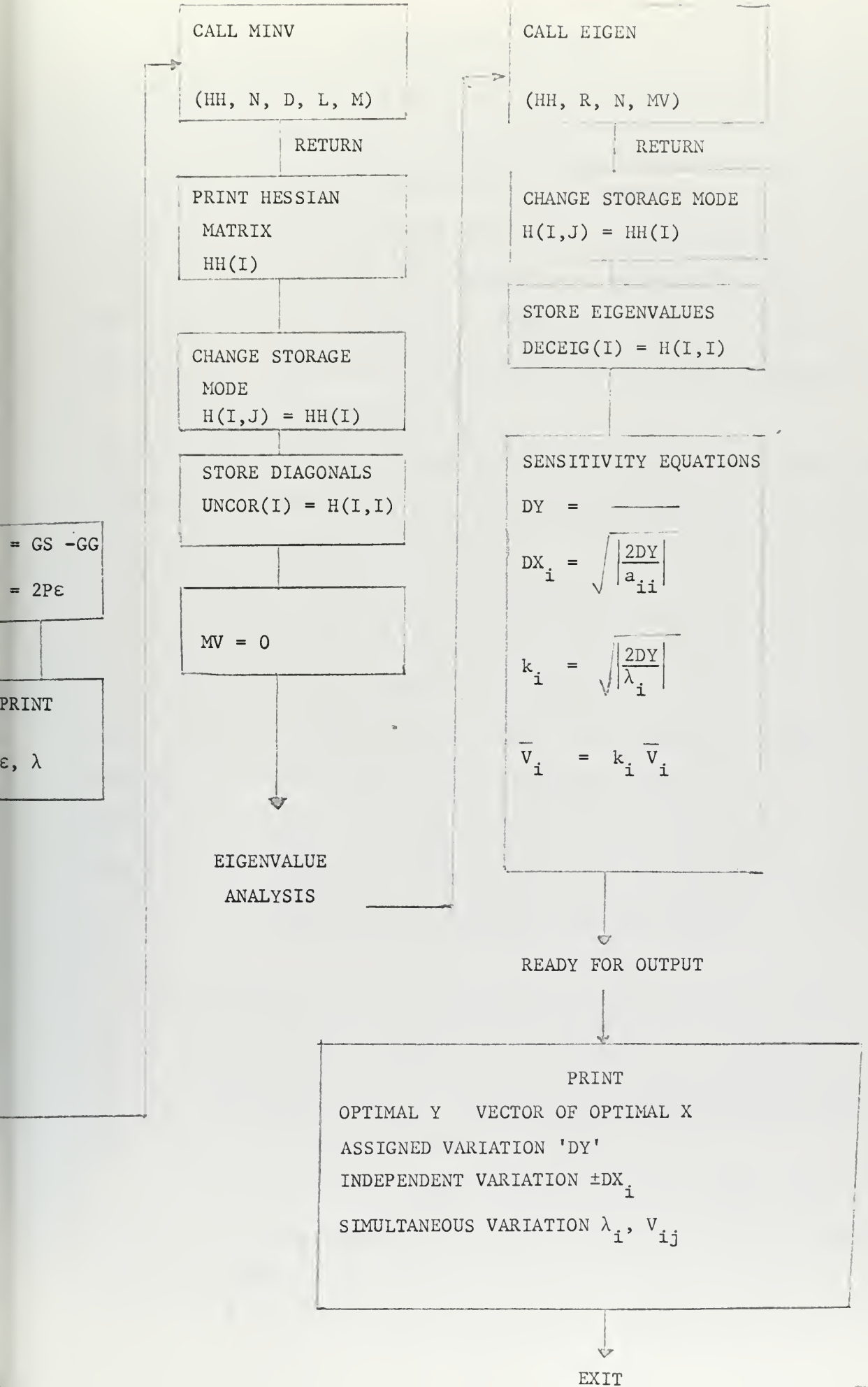
APPENDIX A

This appendix describes the implementation of the variable metric optimization method and matrix inversion and eigenvalue analysis computer programs for the purpose of sensitivity analysis. The input variables and their definitions are shown along with a flow diagram illustrating how the programs were modified to run successively and produce the desired sensitivity data. A typical output format is also given.

The matrix inversion and eigenvalue analysis subroutine listings contain brief descriptions of the methods employed and their references. For a complete description of the computer coded variable metric method consult reference 6.

BLOCK DIAGRAM OF CONTROLLING PROGRAM


START
LOAD
N, STEP, α, β,
NEXP, DELLAM
CHANGE, JPOINT
X(J), X(J)MIN,
X(J)MAX, DELX(J)
TEST
N < 10
FALSE
HALT
X(J) > XMIN(J)
X(J) < XMAX(J)
FALSE
XMIN(J)=X(J)
XMAX(J)=X(J)
TRUE
NGRD = 0
NIMP = 0
INITIAL CALL
MODEL (N,F,X)
NEVAL = 1
FB = F
JFLOW = 0
INITIAL PRINTOUT
NIMP, NGRD, NEVAL,
FB, X(J), J=1, N
OPTIMIZATION LOOP
CALL VARMET
(N, F, X, XMIN, XMAX,
DELX, STEP, α, β,
NEXP, DELLAM, CHANGE,
JPOINT, JFLOW, H)
RETURN
TRUE
JFLOW
N.E.2
FALSE
PRINT OPTIMUM AND
CO-ORDINATES
FB, X(J) J=1, N
TEST CONSTRAINT
G = 0
TRUE
PRINT INVERSE
HESSIAN MATRIX
H(I,J)
CHANGE STORAGE
MODE
HH(I) = H(I,J)
MATRIX
INVERSION


CALL MINV
(HH, N, D, L, M)
RETURN
PRINT HESSIAN MATRIX HH(I)
CHANGE STORAGE MODE H(I,J) = HH(I)
STORE DIAGONALS UNCOR(I) = H(I,I)
MV = 0
EIGENVALUE ANALYSIS
CALL EIGEN
(HH, R, N, MV)
RETURN
CHANGE STORAGE MODE H(I,J) = HH(I)
STORE EIGENVALUES DECEIG(I) = H(I,I)
SENSITIVITY EQUATIONS
DY = ———
DX_i = √|2DY / a_ii|
k_i = √|2DY / λ_i|
V̄_i = k_i V̄_i
READY FOR OUTPUT
PRINT
OPTIMAL Y VECTOR OF OPTIMAL X
ASSIGNED VARIATION 'DY'
INDEPENDENT VARIATION ±DX_i
SIMULTANEOUS VARIATION λ_i, V_ij
EXIT
= GS -GG
= 2Pε
PRINT
ε, λ

Variable Metric Program

Input variables and definitions:

N	=	the number of independent variables
STEP	=	initial step size for X components
ALPHA	=	factor by which step size is increased ($\alpha \geq 1$)
BETA	=	factor by which step size is decreased ($0 \leq \beta \leq 1$)
NEXP	=	limit on number of experiments along a vector line
DELLAM	=	termination criterion for vector search expressed as a range fraction
CHANGE	=	program termination criterion expressed as a range fraction
JPOINT	=	control for type of numerical differentiation desired in gradient subroutine.
		1 = forward difference
		2 = backward difference
		3 = central difference
X(J)	=	vector of initial values for independent variables
XMIN(J)	=	lower bound for each independent variable
XMAX(J)	=	upper bound for each independent variable
DECX(J)	=	step size for each independent variable used in gradient subroutine for numerical differentiation.

There are N + 2 data cards required as inputs for each program execution. The first is an identity card written in any format. The second card contains the first eight input variables listed above in the following format fields. (I10, 3F10.4, I10, 2F10.4, I10)

Each of the N remaining data cards contains the initial value, range and step size of the independent variables according to the following format statement. FORMAT (4F15.5)

A typical output from the variable metric optimization program follows. It should be noted that for the inverse Hessian matrix to be printed properly the array designated H must be dimensioned exactly, i.e. if N = 2 then DIMENSION H (2,2).

```
)BO

      =     2
TEP   =     0.10000
LPHA  =     1.00000
ETA   =     0.50000
XP    =     5
ELLAM =     0.01000
HANGE =     0.00010
POINT =     1


   X           XMIN          XMAX          DELX

 -1.20000    -5.00000      5.00000      0.00100
  1.00000    -5.00000      5.00000      0.00100


NIMP   NGRD  NEVAL       FUNCTION     INDEPENDENT VARIABLES

   0      0      1     0.58400E 01    -0.12000E 01     0.10000E 01
   1      1      4     0.26200E 00    -0.51186E 00    -0.35763E-06
   2      1      6     0.68054E-01    -0.35741E 00    -0.22444E 00
   3      2     12     0.10833E-01     0.14259E 00     0.89546E-01
   4      2     13     0.40146E-12     0.59605E-07    -0.41723E-06
   5      4     25     0.38453E-12     0.63192E-06     0.11936E-07
   6      8     49     0.39664E-13    -0.20230E-06    -0.31673E-08

TIMIZATION COMPLETE AFTER    53 FUNCTION EVALUATIONS
   6      9     53     0.39664E-13    -0.20233E-06    -0.32596E-08
    THE INVERSE HESSIAN MATRIX IS

          1.0000

          0.4999

          0.4999

          0.5001

   HESSIAN MATRIX

          1.9990

         -1.9983

         -1.9983

          3.9973

*ERRCR***     EN-1

   PROGRAMME WAS EXECUTING LINE    65 IN ROUTINE M/PROG WHEN TERMINATION OCC
```

Matrix Inversion and Eigenvalue Analysis

The example output of the variable metric computer code shown previously lists the optimum point and the inverse Hessian matrix at the optimum. Before the matrix inversion subroutine (MINV) may be implemented the upper triangular elements of the symmetric H matrix must be stored in a singly dimensioned array (HH). This was necessary because of the input format utilized in the calling sequence of MINV and was accomplished by inserting a 'DO' loop in the main program.

Once the matrix has been inverted, the elements of the Hessian are printed and the diagonal elements stored for calculation of sensitivity information. Implementation of the eigenvalue analysis subroutine (EIGEN) merely requires defining the constant MV, i.e.

MV = 0 eigenvalues only

MV = 1 eigenvalues and eigenvectors

A dimension statement in the main program for sufficient storage space of the vectors L, M, (utilized by EIGEN) and R (utilized by MINV) is also necessary. All of the required information to construct the table of sensitivity data is now available in the main program. Insertion of the proper equations and output statements completes the modification for sensitivity analysis.

A listing of MINV and EIGEN and an example output format follows.

SUBROUTINE MINV

PURPOSE
INVERT A MATRIX

USAGE
CALL MINV(A,N,D,L,M)

DESCRIPTION OF PARAMETERS
A - INPUT MATRIX, DESTROYED IN COMPUTATION AND REPLACED BY
RESULTANT INVERSE.
N - ORDER OF MATRIX A
D - RESULTANT DETERMINANT
L - WORK VECTOR OF LENGTH N
M - WORK VECTOR OF LENGTH N

REMARKS
MATRIX A MUST BE A GENERAL MATRIX

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
NONE

METHOD
THE STANDARD GAUSS-JORDAN METHOD IS USED. THE DETERMINANT
IS ALSO CALCULATED. A DETERMINANT OF ZERO INDICATES THAT
THE MATRIX IS SINGULAR.

```
      SUBROUTINE MINV(A,N,D,L,M)
      DIMENSION A(1),L(1),M(1)
C     .....................................................................
C
C     IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE
C     C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION
C     STATEMENT WHICH FOLLOWS.
C
C     DOUBLE PRECISION A,D,BIGA,HOLD
C
C     THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS
C     APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS
C     ROUTINE.
C
C     THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO
C     CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  ABS IN STATEMENT
C     10 MUST BE CHANGED TO DABS.
C
C     .....................................................................
C
C     SEARCH FOR LARGEST ELEMENT
C
      D=1.0
      NK=-N
      DO 80 K=1,N
      NK=NK+N
      L(K)=K
      M(K)=K
      KK=NK+K
      BIGA=A(KK)
      DO 20 J=K,N
      IZ=N*(J-1)
      DO 20 I=K,N
      IJ=IZ+I
   10 IF( ABS(BIGA)- ABS(A(IJ))) 15,20,20
   15 BIGA=A(IJ)
      L(K)=I
      M(K)=J
   20 CONTINUE
C
C     INTERCHANGE ROWS
C
      J=L(K)
      IF(J-K) 35,35,25
   25 KI=K-N
      DO 30 I=1,N
      KI=KI+N
      HOLD=-A(KI)
      JI=KI-K+J
      A(KI)=A(JI)
   30 A(JI) =HOLD
C
C     INTERCHANGE COLUMNS
C
   35 I=M(K)
      IF(I-K) 45,45,38
   38 JP=N*(I-1)
      DO 40 J=1,N
      JK=NK+J
```

```
JI=JP+J
HOLD=-A(JK)
A(JK)=A(JI)
A(JI) =HOLD

   DIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS
   CONTAINED IN BIGA)

IF(BIGA) 48,46,48
D=0.0
RETURN
DO 55 I=1,N
IF(I-K) 50,55,50
IK=NK+I
A(IK)=A(IK)/(-BIGA)
CONTINUE

   REDUCE MATRIX

DO 65 I=1,N
IK=NK+I
HOLD=A(IK)
IJ=I-N
DO 65 J=1,N
IJ=IJ+N
IF(I-K) 60,65,60
IF(J-K) 62,65,62
KJ=IJ-I+K
A(IJ)=HOLD*A(KJ)+A(IJ)
CONTINUE

   DIVIDE ROW BY PIVOT

KJ=K-N
DO 75 J=1,N
KJ=KJ+N
IF(J-K) 70,75,70
A(KJ)=A(KJ)/BIGA
CONTINUE

   PRODUCT OF PIVOTS

D=D*BIGA

   REPLACE PIVOT BY RECIPROCAL

A(KK)=1.0/BIGA
CONTINUE

   FINAL ROW AND COLUMN INTERCHANGE

K=N
K=(K-1)
IF(K) 150,150,105
I=L(K)
IF(I-K) 120,120,108
JQ=N*(K-1)
JR=N*(I-1)
DO 110 J=1,N
JK=JQ+J
```

```
OLD=A(JK)
I=JK+J
(JK)=-A(JI)
(JI) =HOLD
=N(K)
F(J-K) 100,100,125
I=K-N
O 130 I=1,N
I=KI+N
OLD=A(KI)
I=KI-K+J
(KI)=-A(JI)
(JI) =HOLD
O TO 100
ETURN
ND
```

SUBROUTINE EIGEN

PURPOSE
COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC MATRIX

USAGE
CALL EIGEN(A,R,N,MV)

DESCRIPTION OF PARAMETERS
A - ORIGINAL MATRIX (SYMMETRIC), DESTROYED IN COMPUTATION. RESULTANT EIGENVALUES ARE DEVELOPED IN DIAGONAL OF MATRIX A IN DESCENDING ORDER.
R - RESULTANT MATRIX OF EIGENVECTORS (STORED COLUMNWISE, IN SAME SEQUENCE AS EIGENVALUES)
N - ORDER OF MATRICES A AND R
MV- INPUT CODE
0 COMPUTE EIGENVALUES AND EIGENVECTORS
1 COMPUTE EIGENVALUES ONLY (R NEED NOT BE DIMENSIONED BUT MUST STILL APPEAR IN CALLING SEQUENCE)

REMARKS
ORIGINAL MATRIX A MUST BE REAL SYMMETRIC (STORAGE MODE=1)
MATRIX A CANNOT BE IN THE SAME LOCATION AS MATRIX R

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
NONE

METHOD
DIAGONALIZATION METHOD ORIGINATED BY JACOBI AND ADAPTED BY VON NEUMANN FOR LARGE COMPUTERS AS FOUND IN 'MATHEMATICAL METHODS FOR DIGITAL COMPUTERS', EDITED BY A. RALSTON AND H.S. WILF, JOHN WILEY AND SONS, NEW YORK, 1962, CHAPTER 7

```
      SUBROUTINE EIGEN(A,R,N,MV)
      DIMENSION A(1),R(1)

     ...............................................................

        IF A DOUBLE PRECISION VERSION OF THIS ROUTINE IS DESIRED, THE
        C IN COLUMN 1 SHOULD BE REMOVED FROM THE DOUBLE PRECISION
        STATEMENT WHICH FOLLOWS.

      DOUBLE PRECISION A,R,ANORM,ANRMX,THR,X,Y,SINX,SINX2,COSX,
     1                 COSX2,SINCS,RANGE

        THE C MUST ALSO BE REMOVED FROM DOUBLE PRECISION STATEMENTS
        APPEARING IN OTHER ROUTINES USED IN CONJUNCTION WITH THIS
        ROUTINE.

        THE DOUBLE PRECISION VERSION OF THIS SUBROUTINE MUST ALSO
        CONTAIN DOUBLE PRECISION FORTRAN FUNCTIONS.  SQRT IN STATEMENTS
        40, 68, 75, AND 78 MUST BE CHANGED TO DSQRT.  ABS IN STATEMENT
        62 MUST BE CHANGED TO DABS. THE CONSTANT IN STATEMENT 5 SHOULD
        BE CHANGED TO 1.0D-12.

     ...............................................................

        GENERATE IDENTITY MATRIX

      RANGE=1.0E-6
      IF(MV-1) 10,25,10
   10 IQ=-N
      DO 20 J=1,N
      IQ=IQ+N
      DO 20 I=1,N
      IJ=IQ+I
      R(IJ)=0.0
      IF(I-J) 20,15,20
   15 R(IJ)=1.0
   20 CONTINUE

        COMPUTE INITIAL AND FINAL NORMS (ANORM AND ANORMX)

      ANORM=0.0
      DO 35 I=1,N
      DO 35 J=I,N
      IF(I-J) 30,35,30
   30 IA=I+(J*J-J)/2
      ANORM=ANORM+A(IA)*A(IA)
   35 CONTINUE
      IF(ANORM) 165,165,40
   40 ANORM=1.414*SQRT(ANORM)
      ANRMX=ANORM*RANGE/FLOAT(N)

        INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR

      IND=0
      THR=ANORM
      THR=THR/FLOAT(N)
      L=1
      M=L+1

        COMPUTE SIN AND COS
```

```
MQ=(M*M-M)/2
LQ=(L*L-L)/2
LM=L+MQ
IF( ABS(A(LM))-THR) 130,65,65
IND=1
LL=L+LQ
MM=M+MQ
X=0.5*(A(LL)-A(MM))
Y=-A(LM)/ SQRT(A(LM)*A(LM)+X*X)
IF(X) 70,75,75
Y=-Y
SINX=Y/ SQRT(2.0*(1.0+( SQRT(1.0-Y*Y))))
SINX2=SINX*SINX
COSX= SQRT(1.0-SINX2)
COSX2=COSX*COSX
SINCS =SINX*COSX

   ROTATE L AND M COLUMNS

ILQ=N*(L-1)
IMQ=N*(M-1)
DO 125 I=1,N
IQ=(I*I-I)/2
IF(I-L) 80,115,80
IF(I-M) 85,115,90
IM=I+MQ
GO TO 95
IM=M+IQ
IF(I-L) 100,105,105
IL=I+LQ
GO TO 110
IL=L+IQ
X=A(IL)*COSX-A(IM)*SINX
A(IM)=A(IL)*SINX+A(IM)*COSX
A(IL)=X
IF(MV-1) 120,125,120
ILR=ILQ+I
IMR=IMQ+I
X=R(ILR)*COSX-R(IMR)*SINX
R(IMR)=R(ILR)*SINX+R(IMR)*COSX
R(ILR)=X
CONTINUE
X=2.0*A(LM)*SINCS
Y=A(LL)*COSX2+A(MM)*SINX2-X
X=A(LL)*SINX2+A(MM)*COSX2+X
A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
A(LL)=Y
A(MM)=X

   TESTS FOR COMPLETION

   TEST FOR M = LAST COLUMN

IF(M-N) 135,140,135
M=M+1
GO TO 60

   TEST FOR L = SECOND FROM LAST COLUMN
```

```
      IF(L-(N-1))  145,150,145
  145 L=L+1
      GO TO 55
  150 IF(IND-1)  160,155,160
  155 IND=0
      GO TO 50

C     COMPARE THRESHOLD WITH FINAL NORM

  160 IF(THR-ANRMX) 165,165,45

C     SORT EIGENVALUES AND EIGENVECTORS

  165 IQ=-N
      DO 185 I=1,N
      IQ=IQ+N
      LL=I+(I*I-I)/2
      JQ=N*(I-2)
      DO 185 J=I,N
      JQ=JQ+N
      MM=J+(J*J-J)/2
      IF(A(LL)-A(MM))  170,185,185
  170 X=A(LL)
      A(LL)=A(MM)
      A(MM)=X
      IF(MV-1)  175,185,175
  175 DO 180 K=1,N
      ILR=IQ+K
      IMR=JQ+K
      X=R(ILR)
      R(ILR)=R(IMR)
  180 R(IMR)=X
  185 CONTINUE
      RETURN
      END
```

TYPICAL OUTPUT FORMAT

THE INVERSE HESSIAN MATRIX IS

0.50546826

1.00514000

1.00514000

2.00354000

HESSIAN MATRIX

826.2998 -415.5432

-415.5432 208.9697

INAL Y VECTOR OF OPTIMAL X

.00000 1.00007 1.00017

SIGNED VARIATION DEL Y = 0.10000

LOWABLE CHANGES IN X VARIED INDEPENDENTLY FOR ASSIGNED VARIATION IN Y

+ OR - DEL X(I)

CS - 0.01094

OR - 0.03094

LLOWABLE CHANGES IN Y VARIED SIMULTANEOUSLY FOR ASSIGNED VARIATION IN Y

IGENVALUE 'K' X EIGENVECTOR

.87000 0.01241 -0.00623

0.39868 0.31772 0.63301